10556437

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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 3	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 4	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 5	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 6	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS 7	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 8	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 9	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 10	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS 11	JUL 28	CA/CAplus patent coverage enhanced
NEWS 12	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 13	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 14	JUL 28	STN Viewer performance improved
NEWS 15	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 16	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 17	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 18	AUG 15	CAplus currency for Korean patents enhanced
NEWS 19	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 20	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 21	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 22	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 23	SEP 29	IFICLS enhanced with new super search field
NEWS 24	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 25	SEP 30	CAS patent coverage enhanced to include exemplified

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                  prophetic substances identified in new Japanese-
                  language patents
 NEWS 26  OCT 07  EPFULL enhanced with full implementation of EPC2000
 NEWS 27  OCT 07  Multiple databases enhanced for more flexible patent
                  number searching

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:59:23 ON 10 OCT 2008

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:59:35 ON 10 OCT 2008
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STRUCTURE FILE UPDATES:    8 OCT 2008  HIGHEST RN 1058803-62-5
DICTIONARY FILE UPDATES:   8 OCT 2008  HIGHEST RN 1058803-62-5

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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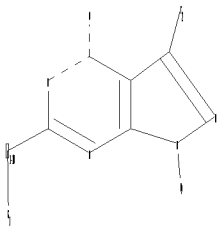
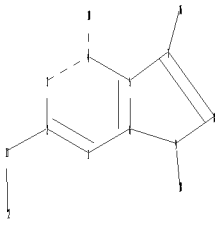
Uploading C:\Program Files\Stnexp\Queries\11556437.str





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10 11 12 16 18
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
2-11 4-10 7-16 9-18 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-16 8-9 9-18 11-12
exact bonds :
2-11

G1:Cy,Ak

G2:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 16:CLASS 18:Atom

L1 STRUCTURE UPLOADED

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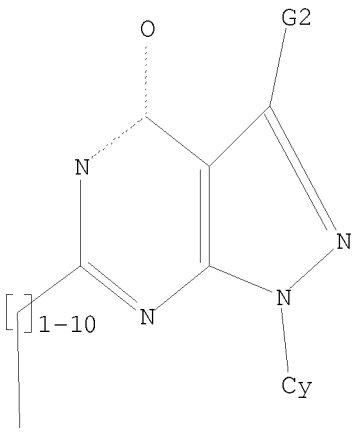
L1 STR



G1 Cy,Ak

G2 H,Me

Structure attributes must be viewed using STN Express query preparation.

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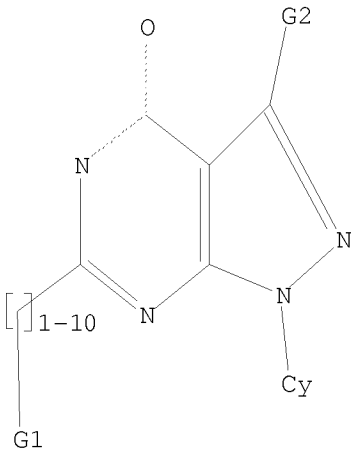

G1 Cy,Ak

G2 H,Me

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 11:06:40 FILE 'REGISTRY'

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SAMPLE SCREEN SEARCH COMPLETED -      405 TO ITERATE

100.0% PROCESSED      405 ITERATIONS                              27 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         6893 TO     9307
PROJECTED ANSWERS:             229 TO      851

L2           27 SEA SSS SAM L1

=> s l1 ful
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100.0% PROCESSED     7965 ITERATIONS                             483 ANSWERS
SEARCH TIME: 00.00.01

L3          483 SEA SSS FUL L1

=> d scan
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L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanamide, 4,5-dihydro-4-oxo-1-phenyl-N-(4-phenyl-2-thiazolyl)-
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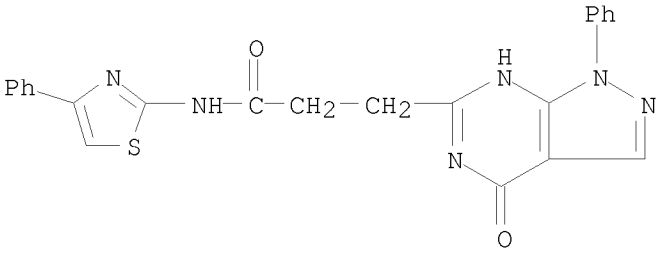
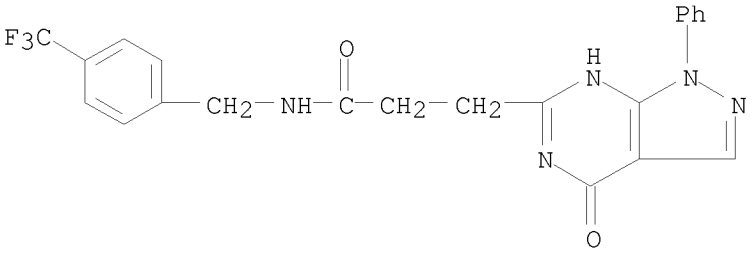


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

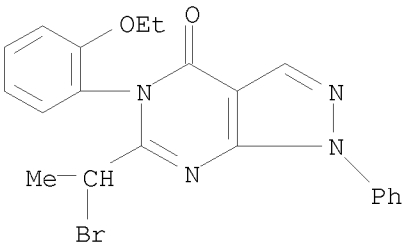
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanamide, 4,5-dihydro-4-oxo-1-phenyl-N-[[4-(trifluoromethyl)phenyl]methyl]-
MF C22 H18 F3 N5 O2



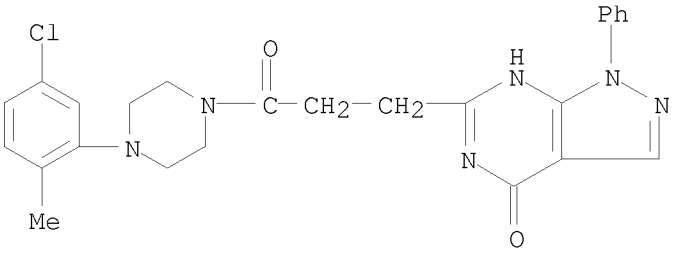
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(1-bromoethyl)-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-
MF C21 H19 Br N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

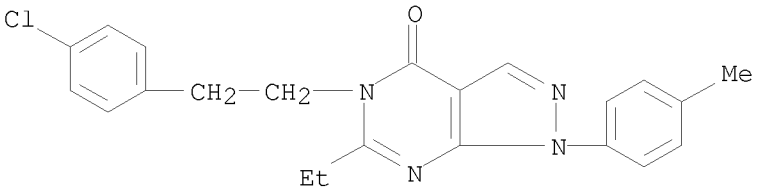
L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[3-[4-(5-chloro-2-methylphenyl)-1-piperazinyl]-3-oxopropyl]-1,5-dihydro-1-phenyl-
MF C25 H25 Cl N6 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

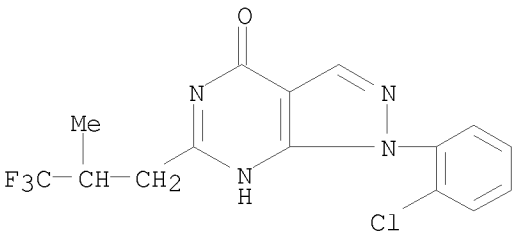
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(4-chlorophenyl)ethyl]-6-ethyl-1,5-dihydro-1-(4-methylphenyl)-
MF C22 H21 Cl N4 O



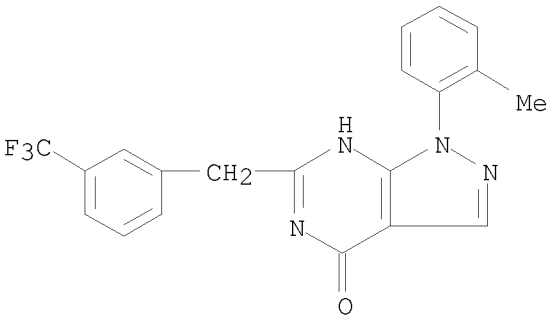
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(3,3,3-trifluoro-2-methylpropyl)-
MF C15 H12 Cl F3 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 483 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[[3-(trifluoromethyl)phenyl]methyl]-
MF C20 H15 F3 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                    184.80     185.01

FILE 'CAPLUS' ENTERED AT 11:08:42 ON 10 OCT 2008
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FILE COVERS 1907 - 10 Oct 2008  VOL 149 ISS 16
FILE LAST UPDATED: 9 Oct 2008  (20081009/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4          29 L3

=> d hist

     (FILE 'HOME' ENTERED AT 10:59:23 ON 10 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 10:59:35 ON 10 OCT 2008
L1              STRUCTURE UPLOADED
L2           27 S L1 SAM
L3          483 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 11:08:42 ON 10 OCT 2008
L4           29 S L3

=> s l4 not (2008/so or 2007/so or 2006/so or 2005/so)
        644762 2008/SO
        965114 2007/SO
        945682 2006/SO
        884917 2005/SO
L5          24 L4 NOT (2008/SO OR 2007/SO OR 2006/SO OR 2005/SO)

=> d l5 ibib hitstr abs 1-24
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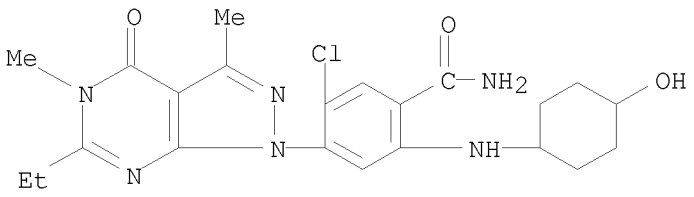
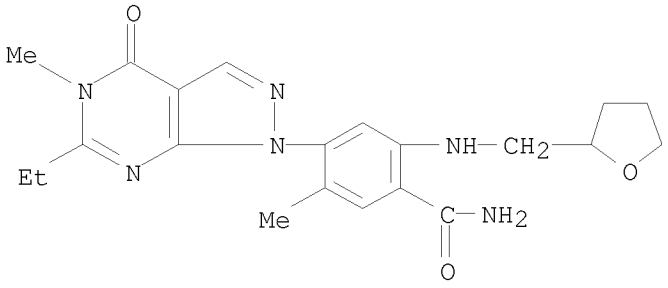
L5 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:256115 CAPLUS
DOCUMENT NUMBER: 148:285203
TITLE: Benzene, pyridine, and pyridazine derivatives as HSP-90 inhibitors and their preparation, pharmaceutical compositions and use in the treatment of proliferative diseases
INVENTOR(S): Huang, Kenneth He; Mangette, John; Barta, Thomas; Hughes, Philip; Hall, Steven E.; Veal, James
PATENT ASSIGNEE(S): Serenex, Inc., USA
SOURCE: PCT Int. Appl., 432pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008024978	A2	20080228	WO 2007-US76770	20070824
WO 2008024978	A3	20080821		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
US 20080119457	A1	20080522	US 2007-844816	20070824

PRIORITY APPLN. INFO.: US 2006-823414P P 20060824
OTHER SOURCE(S): MARPAT 148:285203
IT 1017869-67-8P 1017872-72-8P
RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prophetic drug candidate; preparation of benzene, pyridine, and pyridazine derivs. as HSP-90 inhibitors useful in the treatment of proliferative diseases)
RN 1017869-67-8 CAPLUS
CN Benzamide, 5-chloro-4-(6-ethyl-4,5-dihydro-3,5-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-2-[(4-hydroxycyclohexyl)amino]- (CA INDEX NAME)



RN 1017872-72-8 CAPLUS
CN Benzamide, 4-(6-ethyl-4,5-dihydro-5-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-5-methyl-2-[[(tetrahydro-2-furanyl)methyl]amino]- (CA INDEX NAME)



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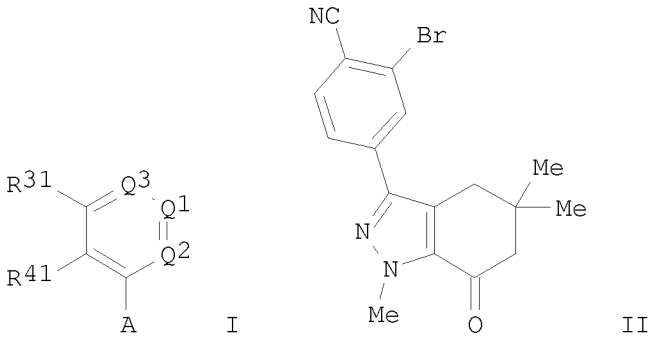

AB Disclosed are compds. and pharmaceutically acceptable salts of formula I. Compds. of formula I are useful in the treatment of diseases and/or conditions related to cell proliferation, such as cancer, inflammation, arthritis, angiogenesis, or the like. Also disclosed are pharmaceutical compns. comprising compds. of the invention and methods of treating the aforementioned conditions using such compds. Compds. of formula I wherein Q1, Q2 and Q3 are independently N and CRx, provided that no more than two of Q1, Q2 and Q3 are N; each Rx is independently H, halo, (hetero)aryl, C1-6 (halo)alkyl, etc.; A is (un)substituted (hetero)bicyclic derivative and (un)substituted 5-membered (hetero)cyclic ring; R31 and R41 are independently H, halo, C1-15 (hetero)alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by epoxidn. of 4,4-dimethylcyclohex-2-enone; the resulting 5,5-dimethyl-7-oxabicyclo[4.1.0]heptan-2-one underwent addition of methanol followed by elimination to give 2-methoxy-4,4-dimethylcyclohex-2-enone, which underwent acylation with 3-bromo-4-cyanobenzoyl chloride to give 2-bromo-4-(3-methoxy-5,5-dimethyl-2-oxocyclohex-3-enecarbonyl)benzonitrile, which underwent cyclization with methylhydrazine

to give compound II. All the invention compds. were evaluated for their HSP-90 inhibitory activity (some data given).

L5 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:729227 CAPLUS
DOCUMENT NUMBER: 147:143456
TITLE: Fused pyrimidones and thiopyrimidones, and their preparation, pharmaceutical compositions and use in killing or reducing cancer cell proliferation
INVENTOR(S): Venkat, Raj Gopal; Qi, Longwu; Pierce, Michael; Robbins, Paul B.; Sahasrabudhe, Sudhir R.; Selliah, Robert
PATENT ASSIGNEE(S): Prolexys Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 77pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007076085	A2	20070705	WO 2006-US49168	20061222
WO 2007076085	A3	20070823		

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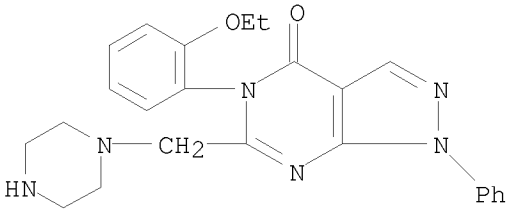
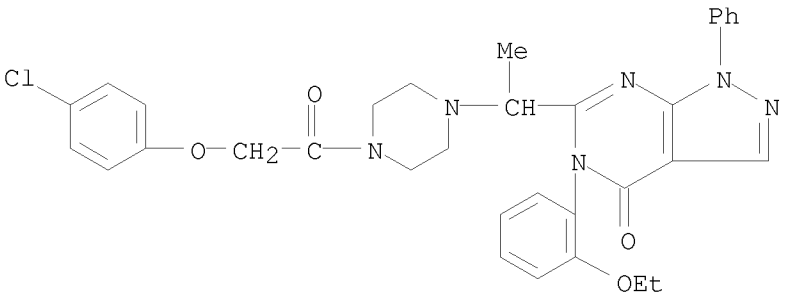
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-753916P P 20051222
US 2006-834989P P 20060727
OTHER SOURCE(S): MARPAT 147:143456
IT 943430-97-5P 943431-00-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of fused pyrimidone and thiopyrimidone compds. useful in killing or reducing cancer cell proliferation)
RN 943430-97-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-6-(1-piperazinylmethyl)- (CA INDEX NAME)



RN 943431-00-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[1-[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]ethyl]-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl- (CA INDEX NAME)



IT 943431-16-1P 943431-17-2P 943431-18-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused pyrimidone and thiopyrimidone compds. useful in killing or reducing cancer cell proliferation)

RN 943431-16-1 CAPLUS
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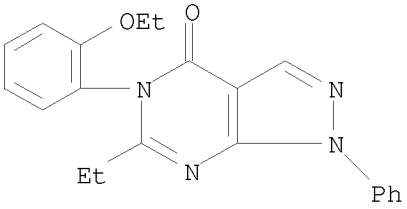

RN 943431-17-2 CAPLUS
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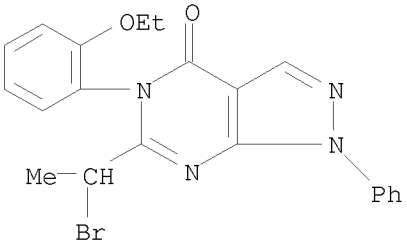
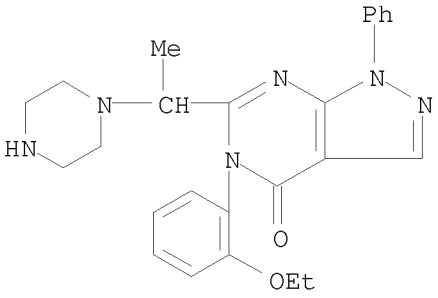


RN 943431-18-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-6-[1-(1-piperazinyl)ethyl]- (CA INDEX NAME)



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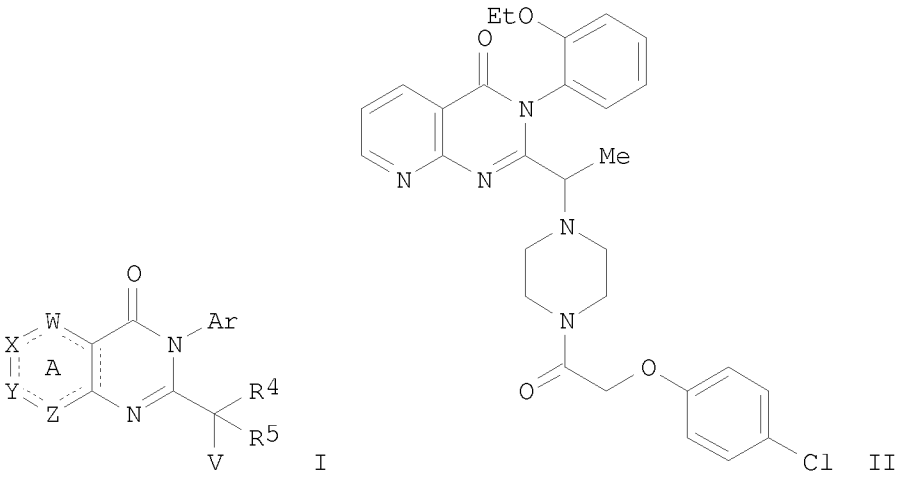


I II

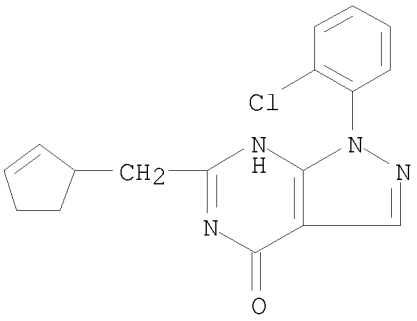
AB Compds. represented by structural formula I: are useful, for example, in the effective killing or reduction in rate of proliferation of cancer cells, such as in patients suffering from cancer. In addition to the compds. themselves, the invention provides pharmaceutical compns. of the compds. and method of treatment using the compds. Compds. of formula I wherein ring A is optionally substituted: W is absent, C, N, S and O; X, Y and Z is C, N, S and O where at least one of X, Y and Z is N if W is C; Ar is (un)substituted phenyl; R4 and R5 are independently H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted heterocyclyl, and (un)substituted aryl; V i substituted amine and cyclic amines; dotted lines are single and double bonds; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure. All the invention compds. were evaluated for their ability to kill or reduce cancer cell proliferation.

L5 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1253041 CAPLUS
DOCUMENT NUMBER: 146:757
TITLE: Use of pyrazolopyrimidine compounds for the treatment of cardiovascular diseases
INVENTOR(S): Hendrix, Martin; Wunder, Frank; Tersteegen, Adrian; Stasch, Johannes-Peter
PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
SOURCE: PCT Int. Appl., 48pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006125548	A1	20061130	WO 2006-EP4591	20060516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102005024493	A1	20061130	DE 2005-102005024493	20050527
EP 1888076	A1	20080220	EP 2006-753634	20060516
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: DE 2005-102005024493A 20050527
WO 2006-EP4591 W 20060516

OTHER SOURCE(S): MARPAT 146:757
IT 794568-65-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pyrazolopyrimidine compds. for treatment of cardiovascular diseases)
RN 794568-65-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)



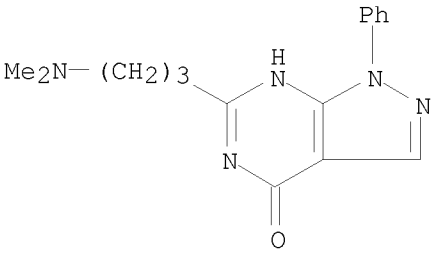
AB The invention discloses the use of pyrazolopyrimidine compds. for producing medicaments drugs for treating cardiovascular diseases.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:471917 CAPLUS
DOCUMENT NUMBER: 144:488675
TITLE: Preparation of 1,4-substituted pyrazolopyrimidines as kinase inhibitors, particularly EphB4 inhibitors
INVENTOR(S): Schmiedeberg, Niko; Furet, Pascal; Imbach, Patricia; Holzer, Philipp
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006050946	A1	20060518	WO 2005-EP12045	20051110
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005303965	A1	20060518	AU 2005-303965	20051110
CA 2585660	A1	20060518	CA 2005-2585660	20051110
EP 1812441	A1	20070801	EP 2005-819276	20051110
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 101098873	A	20080102	CN 2005-80046410	20051110
JP 2008519790	T	20080612	JP 2007-540577	20051110
IN 2007DN03269	A	20070831	IN 2007-DN3269	20070501
US 20080096868	A1	20080424	US 2007-718730	20070507
MX 200705644	A	20070605	MX 2007-5644	20070510
KR 2007084191	A	20070824	KR 2007-710778	20070511
PRIORITY APPLN. INFO.:			GB 2004-25035 A	20041112
			WO 2005-EP12045 W	20051110

OTHER SOURCE(S): MARPAT 144:488675
IT 887327-53-9P, 6-(3-Dimethylaminopropyl)-1-phenyl-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 1,4-substituted pyrazolopyrimidines as EphB4 inhibitors)
RN 887327-53-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[3-(dimethylamino)propyl]-1,5-dihydro-1-phenyl- (CA INDEX NAME)



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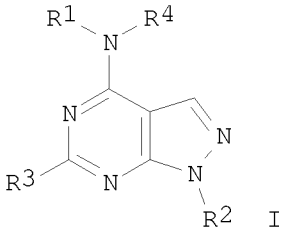

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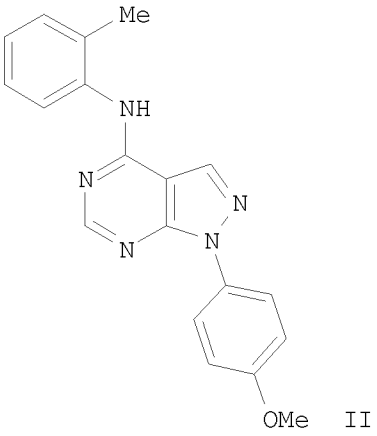


II

AB The invention is related to 1,4-substituted pyrazolopyrimidines I [R1 = (un)substituted Ph; R2 = (un)substituted aryl; R3 = H, (un)substituted alkyl, aryl, heterocyclyl; R4 = H, (un)substituted alkyl], and their pharmaceutically acceptable salts where one or more salt-forming groups are present, pharmaceuticals comprising them, and their use in the diagnosis and treatment or manufacture of a pharmaceutical formulation for the treatment of a disease that depends on inadequate activity of a protein kinase, especially a protein tyrosine kinase, preferably one or more of c-Abl, c-Src and/or especially Ephrin B4 receptor (EphB4) kinases; and/or one or more altered or mutated forms of any one or more of these, e.g. those forms that result in conversion of the resp. proto-oncogene into an oncogene,

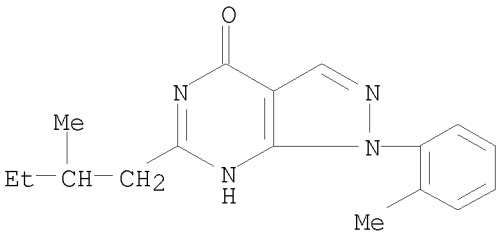
such as constitutively activated Bcr-Abl or v-Src. The invention is also related to the preparation of pyrazolopyrimidines I. Thus, II•TFA was prepared starting from 4-methoxyphenylhydrazine•xHCl and (ethoxymethylene)malononitrile. Pyrazolopyrimidine II•TFA inhibited EphB4 (Ic50 = 0.16 μmol/l).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

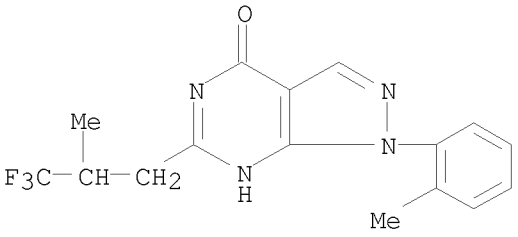
L5 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:996183 CAPLUS
DOCUMENT NUMBER: 141:424206
TITLE: Preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics.
INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099211	A1	20041118	WO 2004-EP4455	20040428
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004142	A1	20041125	DE 2004-102004004142	20040128
AU 2004235915	A1	20041118	AU 2004-235915	20040428
CA 2524900	A1	20041118	CA 2004-2524900	20040428
EP 1626971	A1	20060222	EP 2004-729876	20040428
R: DE, ES, FR, GB, IT				
JP 2006525966	T	20061116	JP 2006-505294	20040428
US 20070105876	A1	20070510	US 2005-556224	20051109
IN 2005DN05418	A	20070928	IN 2005-DN5418	20051124
PRIORITY APPLN. INFO.:			DE 2003-10320784 A	20030509
			DE 2003-10336183 A	20030807
			DE 2004-102004004142A	20040128
			WO 2004-EP4455 W	20040428

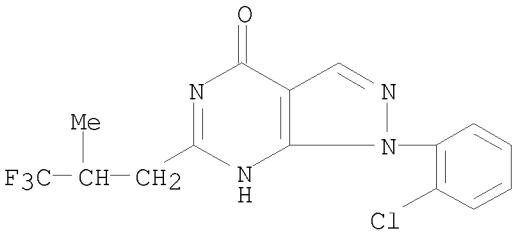
OTHER SOURCE(S): MARPAT 141:424206
IT 794568-84-6P 794568-87-9P 794568-90-4P
794568-94-8P
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)
RN 794568-84-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(2-methylbutyl)-1-(2-methylphenyl)- (CA INDEX NAME)



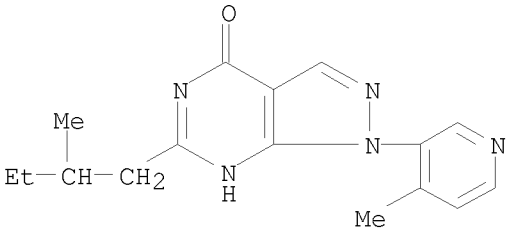
RN 794568-87-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)



RN 794568-90-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)



RN 794568-94-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(2-methylbutyl)-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

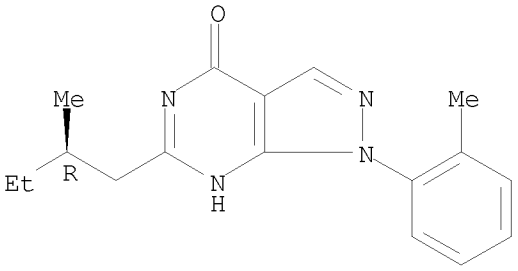


IT 794568-85-7P 794568-86-8P 794568-88-0P
794568-89-1P 794568-91-5P 794568-92-6P

794568-95-9P 794568-96-0P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

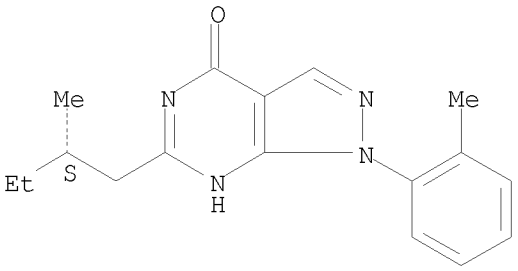
RN 794568-85-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



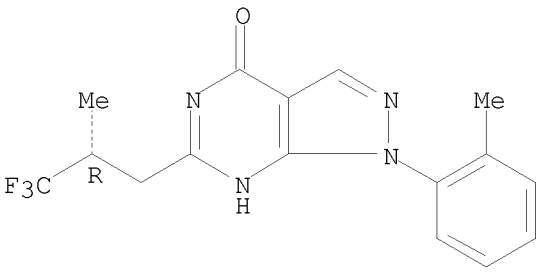
RN 794568-86-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



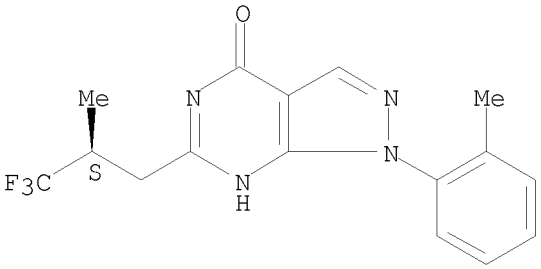
RN 794568-88-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



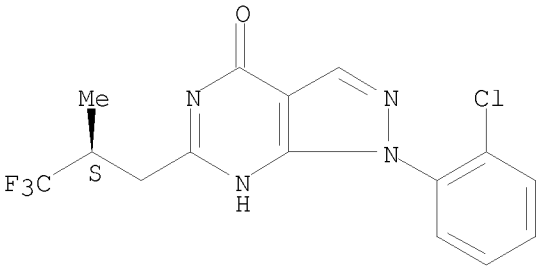
RN 794568-89-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



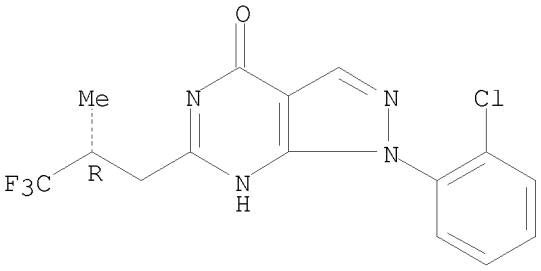
RN 794568-91-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



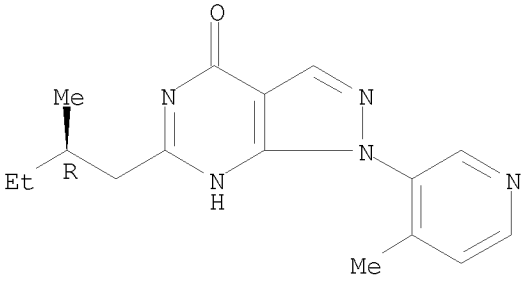
RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



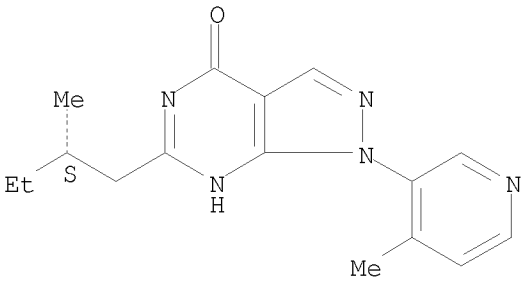
RN 794568-95-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 794568-96-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



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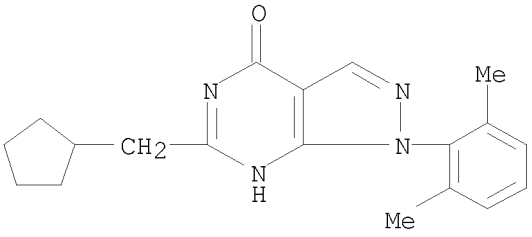
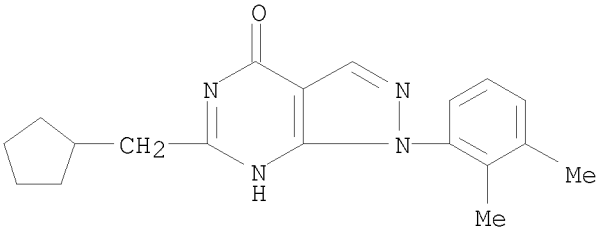
794568-56-2P 794568-57-3P 794568-58-4P
794568-59-5P 794568-60-8P 794568-61-9P
794568-62-0P 794568-63-1P 794568-64-2P
794568-65-3P 794568-66-4P 794568-67-5P
794568-68-6P 794568-69-7P 794568-70-0P
794568-71-1P 794568-72-2P 794568-73-3P

794568-74-4P 794568-75-5P 794568-76-6P
794568-77-7P 794568-78-8P 794568-79-9P
794568-80-2P 794568-81-3P 794568-82-4P
794568-83-5P 794568-93-7P 794568-97-1P
794568-98-2P 794568-99-3P 794569-00-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

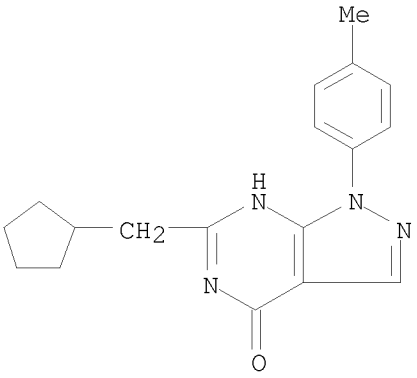
RN 794568-50-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



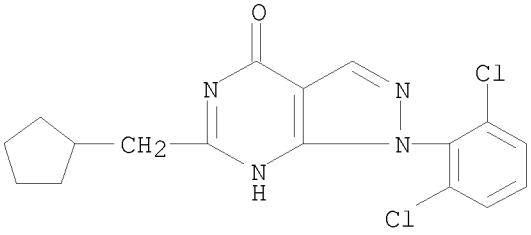
RN 794568-51-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



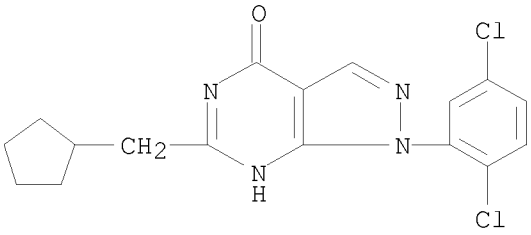
RN 794568-52-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methylphenyl)- (CA INDEX NAME)



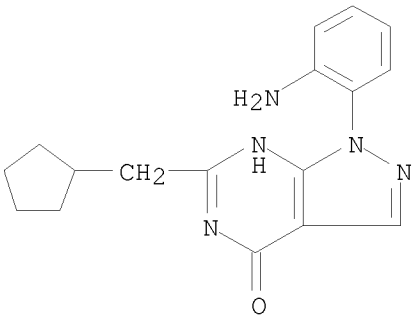
RN 794568-53-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



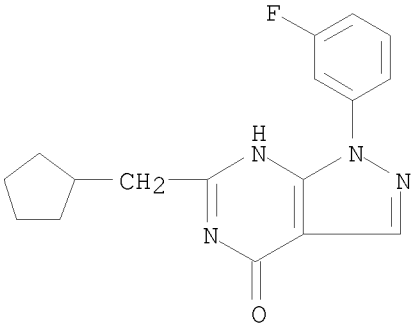
RN 794568-54-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



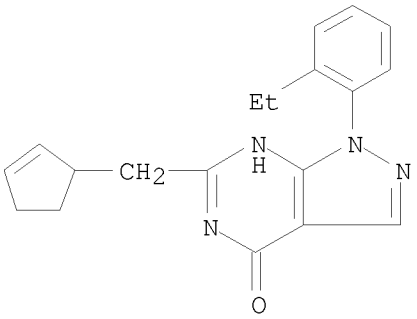
RN 794568-55-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-aminophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



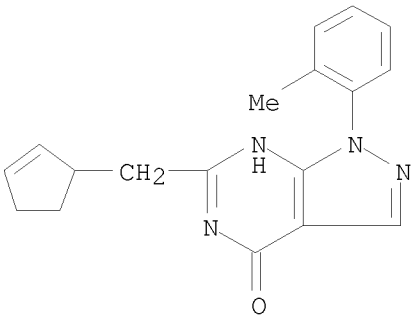
RN 794568-56-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(3-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)



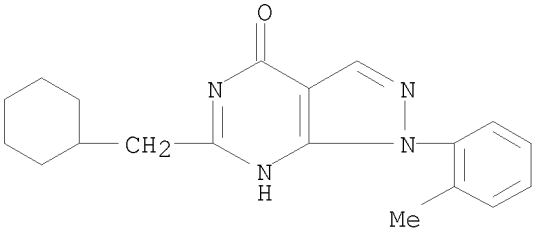
RN 794568-57-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)



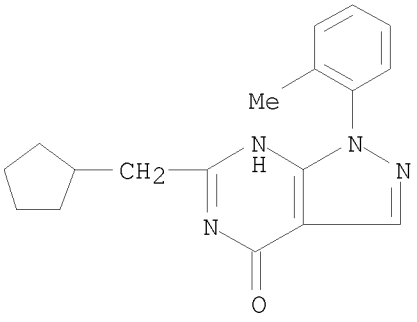
RN 794568-58-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



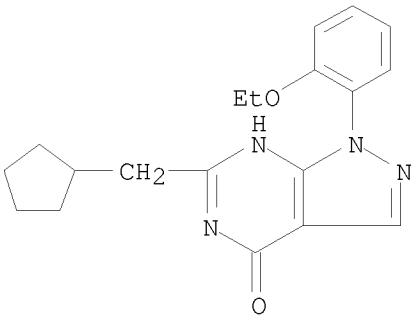
RN 794568-59-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



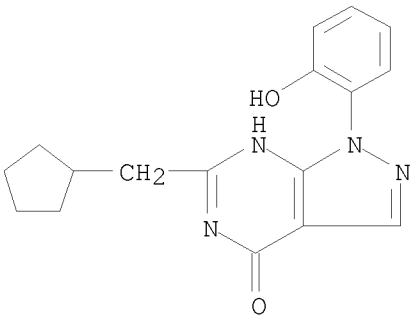
RN 794568-60-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



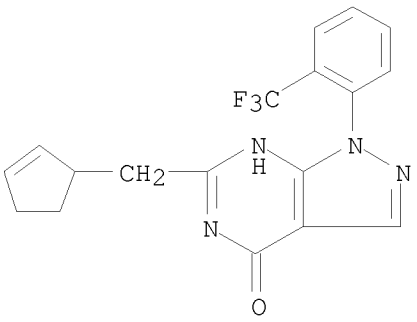
RN 794568-61-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2-ethoxyphenyl)-1,5-dihydro- (CA INDEX NAME)



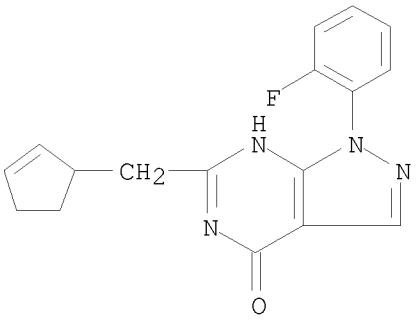
RN 794568-62-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-hydroxyphenyl)- (CA INDEX NAME)



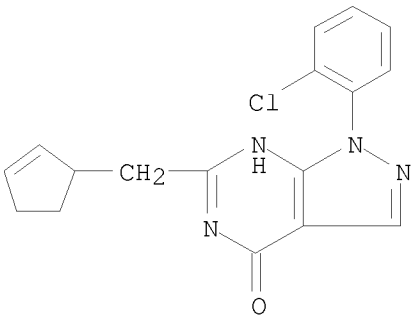
RN 794568-63-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



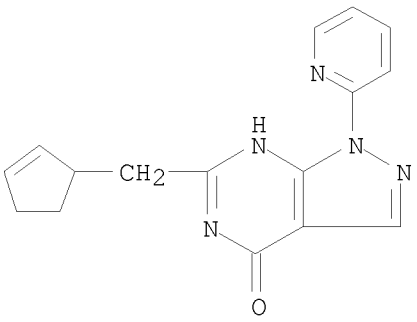
RN 794568-64-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(2-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)



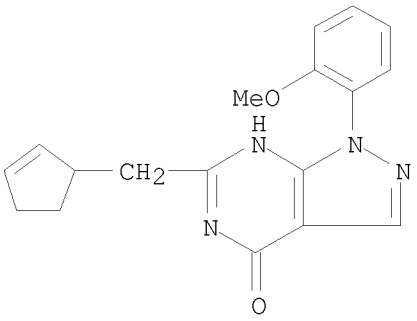
RN 794568-65-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)



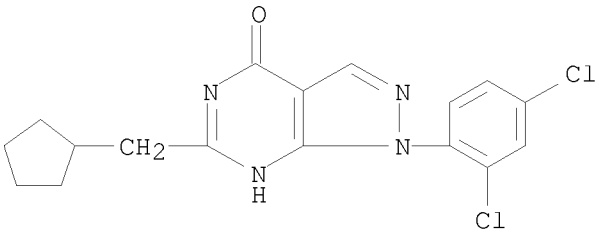
RN 794568-66-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)



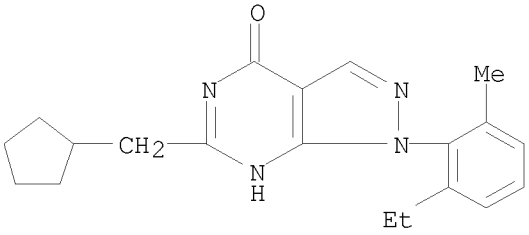
RN 794568-67-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX NAME)



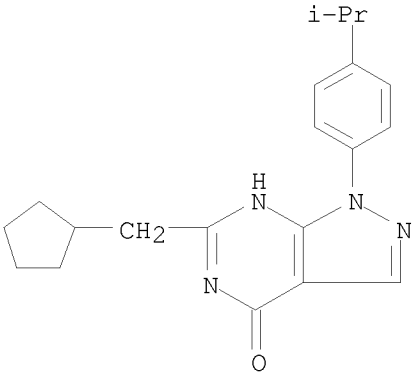
RN 794568-68-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



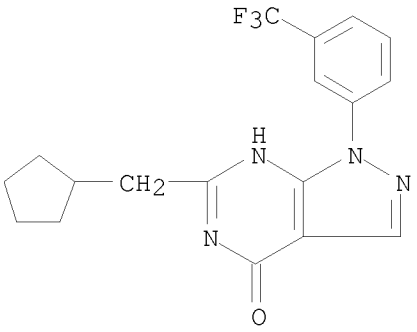
RN 794568-69-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2-ethyl-6-methylphenyl)-1,5-dihydro- (CA INDEX NAME)



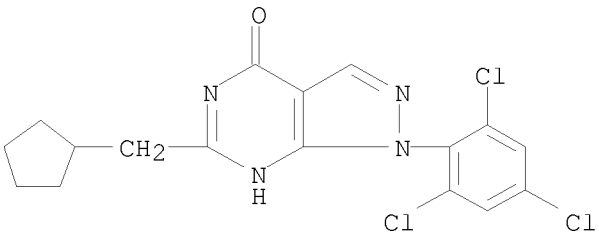
RN 794568-70-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



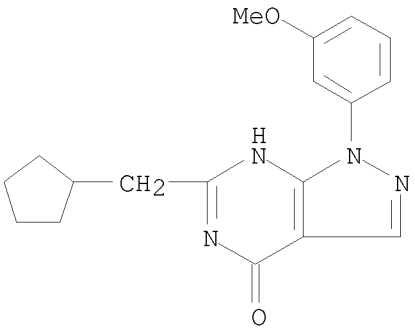
RN 794568-71-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



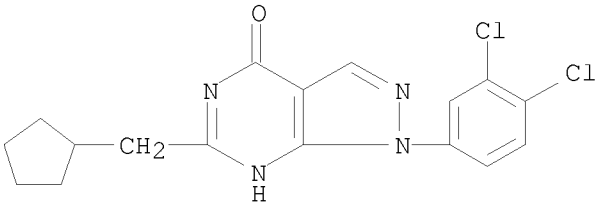
RN 794568-72-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



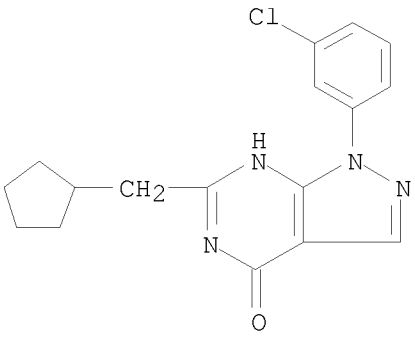
RN 794568-73-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(3-methoxyphenyl)- (CA INDEX NAME)



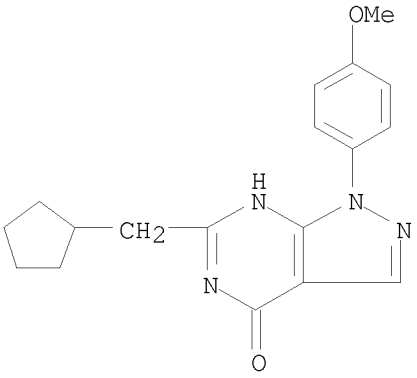
RN 794568-74-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(3,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



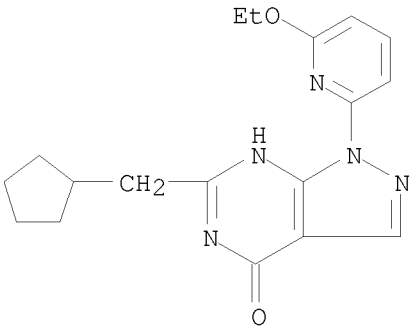
RN 794568-75-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(3-chlorophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



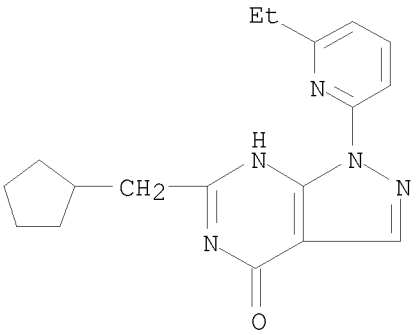
RN 794568-76-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methoxyphenyl)- (CA INDEX NAME)



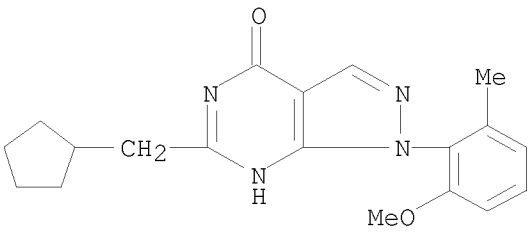
RN 794568-77-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(6-ethoxy-2-pyridinyl)-1,5-dihydro- (CA INDEX NAME)



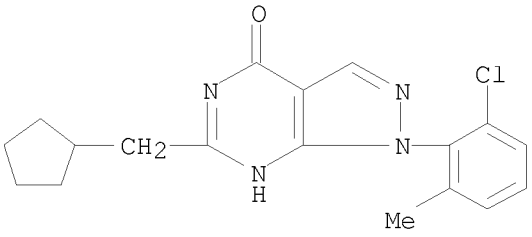
RN 794568-78-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(6-ethyl-2-pyridinyl)-1,5-dihydro- (CA INDEX NAME)



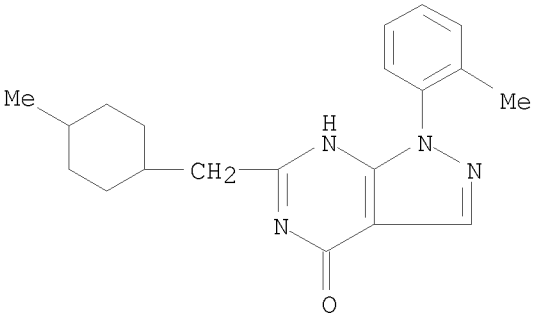
RN 794568-79-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methoxy-6-methylphenyl)- (CA INDEX NAME)



RN 794568-80-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chloro-6-methylphenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)

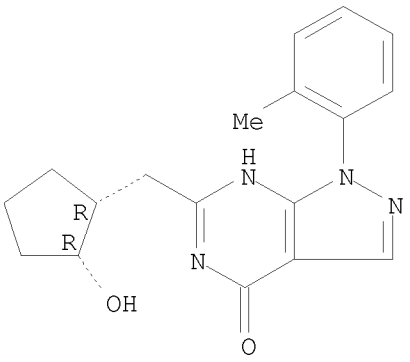


RN 794568-81-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(4-methylcyclohexyl)methyl]-1-(2-methylphenyl)- (CA INDEX NAME)



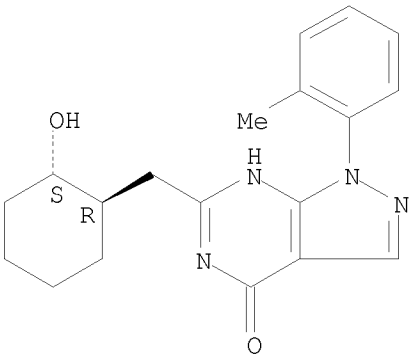
RN 794568-82-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[[(1R,2R)-2-hydroxycyclopentyl]methyl]-1-(2-methylphenyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.

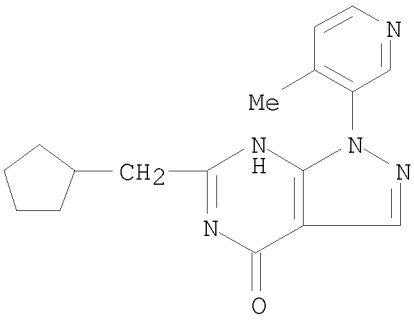


RN 794568-83-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[[(1R,2S)-2-hydroxycyclohexyl]methyl]-1-(2-methylphenyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.

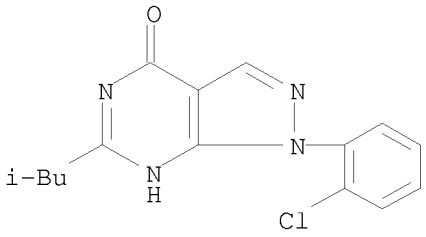


RN 794568-93-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

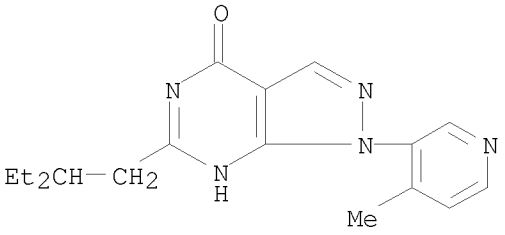


RN 794568-97-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(2-

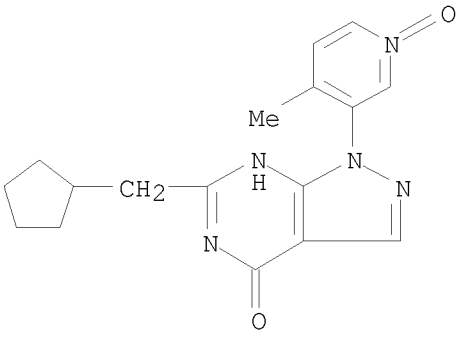
methylpropyl)- (CA INDEX NAME)



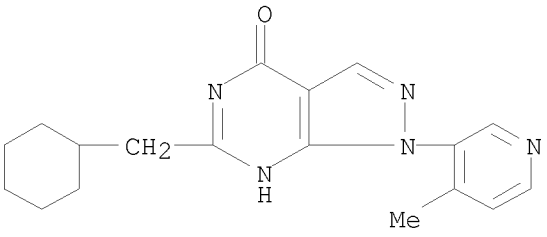
RN 794568-98-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-ethylbutyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)



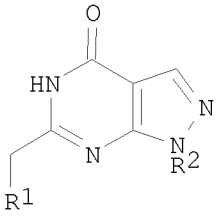
RN 794568-99-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methyl-1-oxido-3-pyridinyl)- (CA INDEX NAME)



RN 794569-00-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)



GI



I

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = (substituted) Ph, heteroaryl], were prepared Thus, reflux of 5-amino-1-(2-methylphenyl)-1H-pyrazole-4-carboxamide (preparation given) with Et cyclopentylacetate and NaH in EtOH overnight gave 30% 6-cyclopentylmethyl-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2004:996182 CAPLUS
DOCUMENT NUMBER: 141:410967
TITLE: Preparation of 6-arylmethylpyrazolopyrimidines as PDE9A inhibitors for the treatment of Alzheimer's disease
INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099210	A1	20041118	WO 2004-EP4412	20040427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10320785	A1	20041125	DE 2003-10320785	20030509
CA 2524898	A1	20041118	CA 2004-2524898	20040427
EP 1628980	A1	20060301	EP 2004-739107	20040427
R: DE, ES, FR, GB, IT				
JP 2006525963	T	20061116	JP 2006-505276	20040427
US 20070161662	A1	20070712	US 2006-556437	20061010
PRIORITY APPLN. INFO.:			DE 2003-10320785 A	20030509
			WO 2004-EP4412 W	20040427

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6-(3-Chlorobenzyl)-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-92-2P, 1-(2-Methylphenyl)-6-(2-pyridinylmethyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-93-3P, 6-(3-Chlorobenzyl)-1-(2-ethylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-94-4P, 6-(3-Chlorobenzyl)-1-(2-trifluoromethylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-95-5P, 6-(3-Chlorobenzyl)-1-(2-fluorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-96-6P, 6-(3-Chlorobenzyl)-1-(2-chlorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-97-7P, 6-(3-Chlorobenzyl)-1-(2-pyridinyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-98-8P, 6-(3-Chlorobenzyl)-1-(2-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylmethylpyrazolopyrimidines as PDE9A inhibitors for the treatment of Alzheimer's disease)

RN 792952-76-2 CAPLUS
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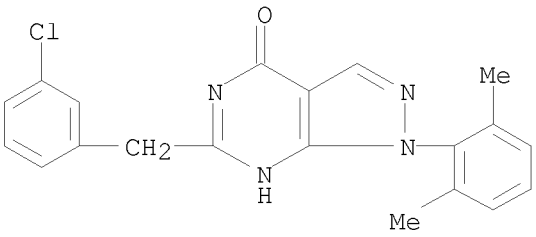
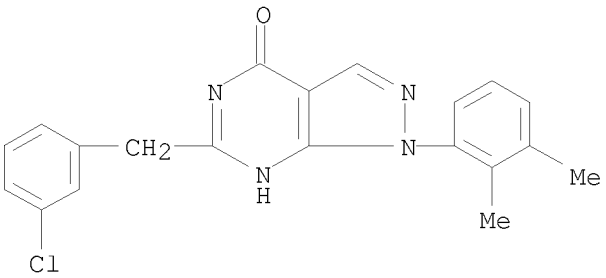


RN 792952-77-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



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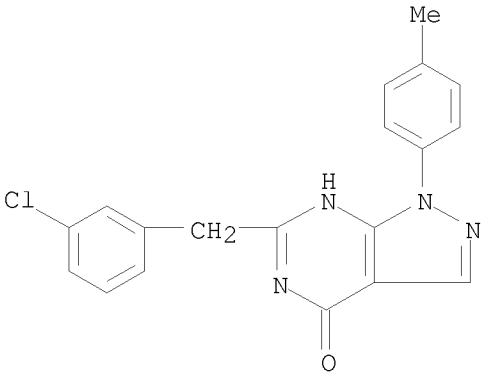
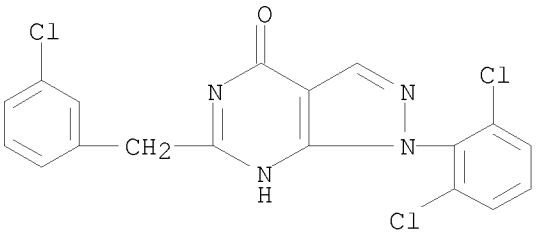
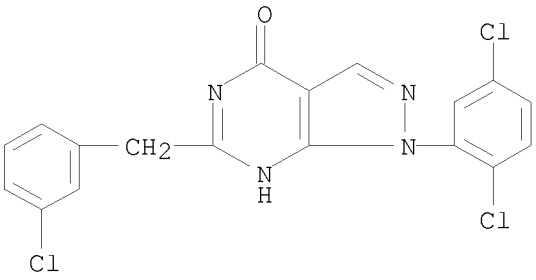


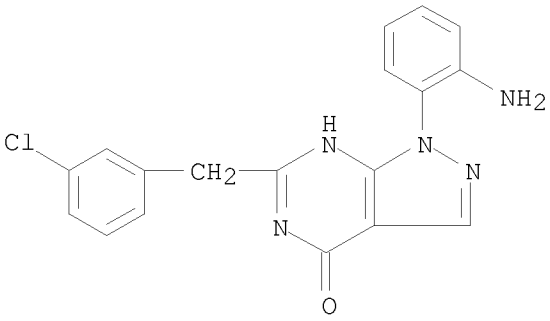
RN 792952-79-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



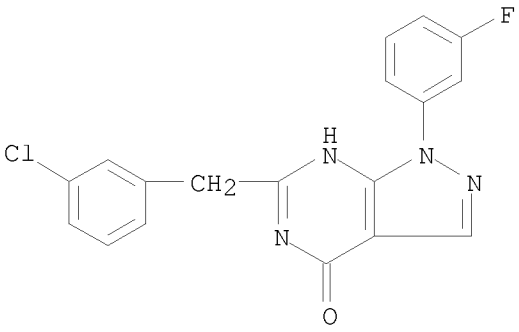
RN 792952-80-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



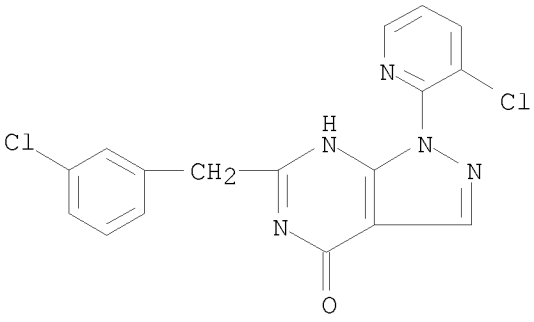
RN 792952-81-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-aminophenyl)-6-[(3-chlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



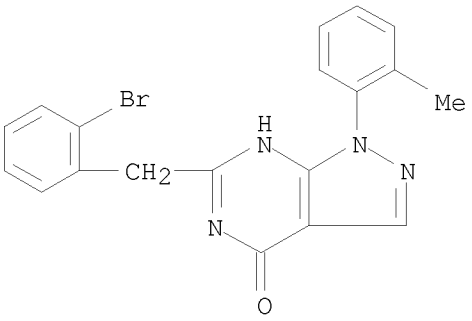
RN 792952-82-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(3-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)



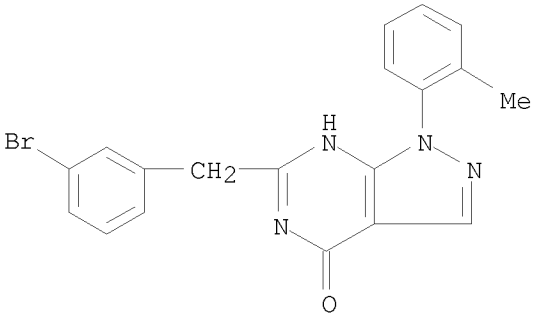
RN 792952-83-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(3-chloro-2-pyridinyl)-1,5-dihydro- (CA INDEX NAME)



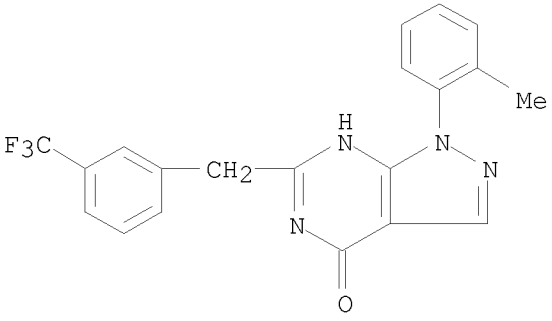
RN 792952-84-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(2-bromophenyl)methyl]-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



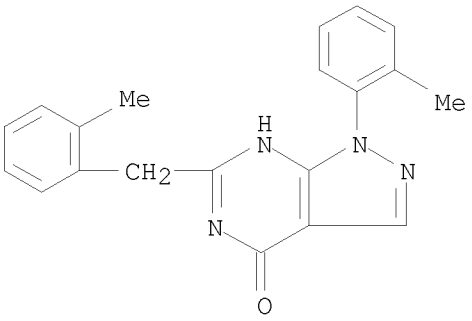
RN 792952-85-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-bromophenyl)methyl]-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



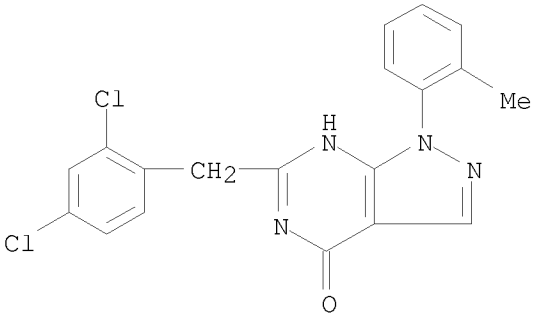
RN 792952-86-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)



RN 792952-87-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(2-methylphenyl)methyl]- (CA INDEX NAME)



RN 792952-88-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(2,4-dichlorophenyl)methyl]-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



RN 792952-89-7 CAPLUS
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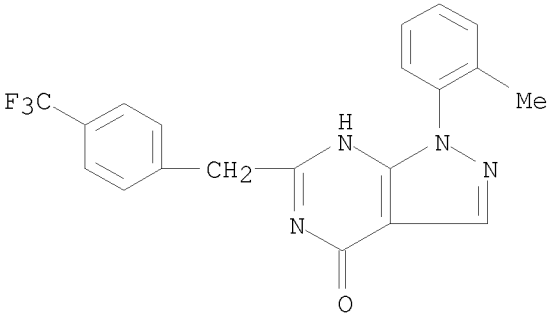
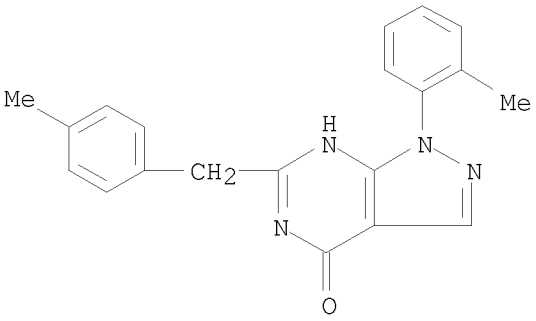
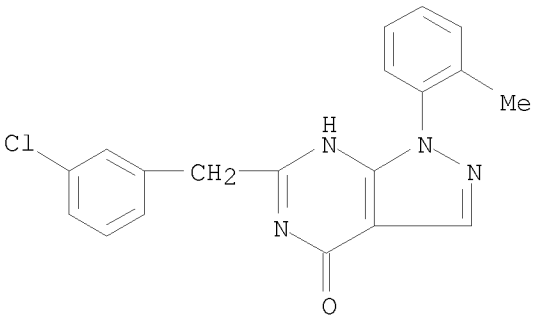


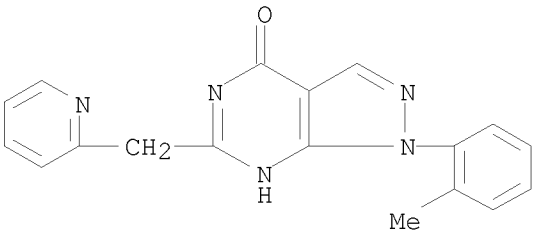
RN 792952-90-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-[(4-methylphenyl)methyl]- (CA INDEX NAME)



RN 792952-91-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



RN 792952-92-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-(2-pyridinylmethyl)- (CA INDEX NAME)



RN 792952-93-3 CAPLUS
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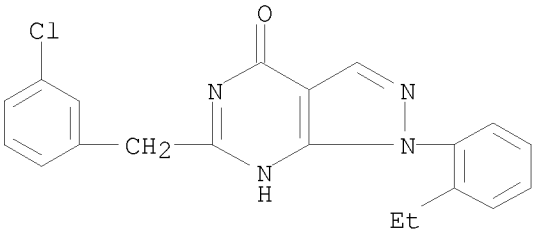

RN 792952-94-4 CAPLUS
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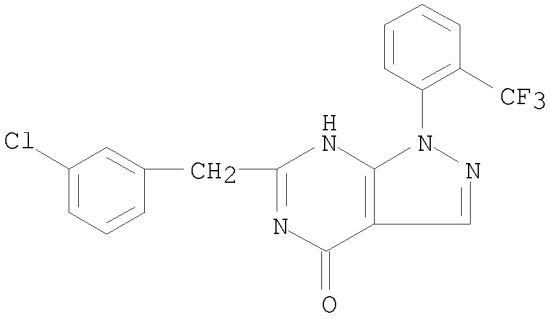

RN 792952-95-5 CAPLUS
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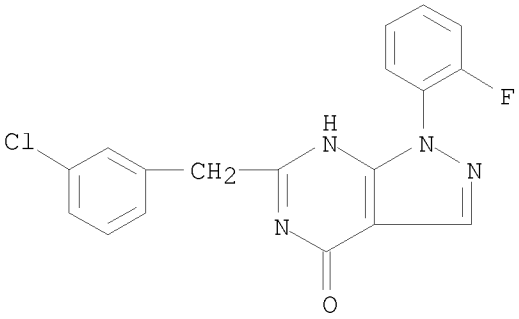

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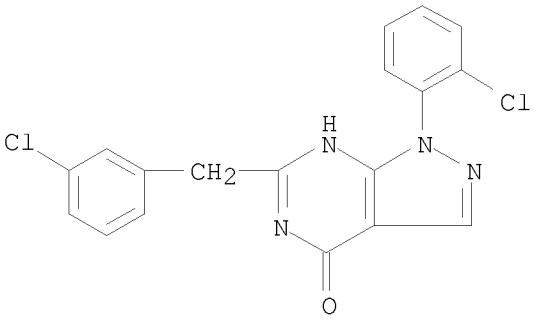

RN 792952-97-7 CAPLUS
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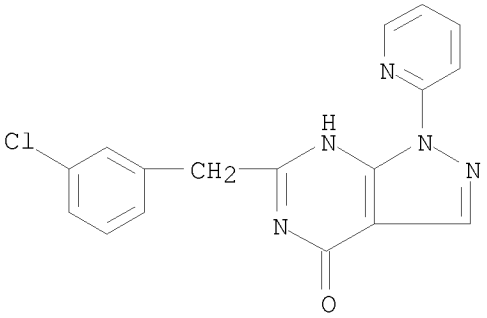

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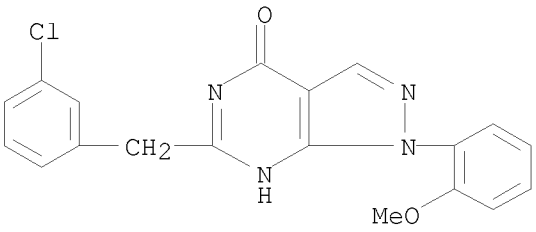

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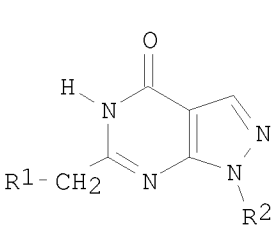

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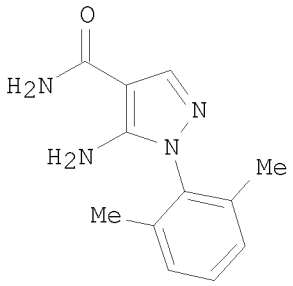

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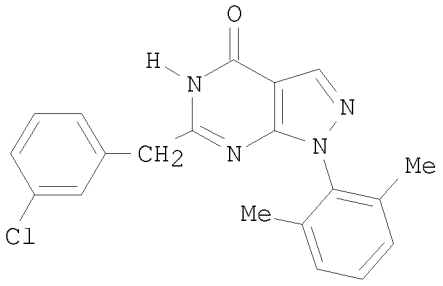

III

AB Title compds. I [R1 = (un)substituted Ph, pyridyl, thiophenyl, etc.; (un)substituted Ph, heteroaryl] and their pharmaceutically acceptable salts were prepared For example, condensation-cyclization of 3-chlorophenylacetic acid Me ester and aminopyrazole II, e.g., prepared from 2,3-dimethylphenylhydrazine hydrochloride and (ethoxymethylene)propanedinitrile, afforded pyrazolopyrimidine III in 37% yield. In human guanosine cyclic 3,5'-phosphate phosphodiesterase (PDE9A) inhibition assays, 4-examples of compds. I exhibited IC50 values ranging from <30-64 nM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:934326 CAPLUS
DOCUMENT NUMBER: 141:395571
TITLE: Preparation of pyrazolopyrimidinones as phosphodiesterase 9 (PDE9) inhibitors for treating type 2 diabetes, metabolic syndrome, and cardiovascular disease.
INVENTOR(S): Bell, Andrew Simon; Deninno, Michael Paul; Palmer, Michael John; Visser, Michael Scott
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040220186	A1	20041104	US 2004-828485	20040420
WO 2004096811	A1	20041111	WO 2004-IB1796	20040421
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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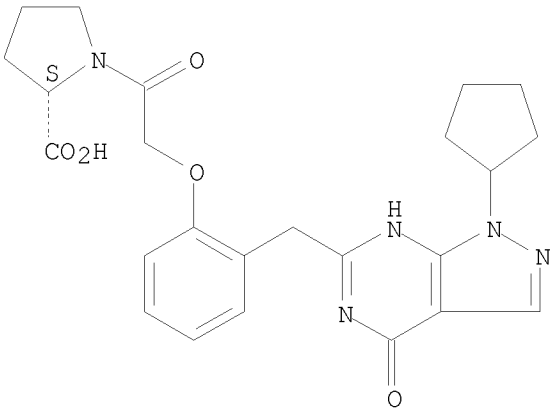
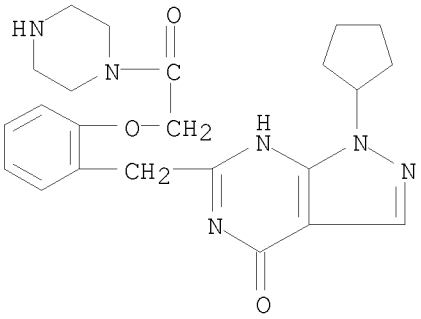
NL 1026091	A1	20041102	NL 2004-1026091	20040429
NL 1026091	C2	20050526		

PRIORITY APPLN. INFO.: US 2003-466639P P 20030430
US 2004-828485 A 20040420
OTHER SOURCE(S): MARPAT 141:395571
IT 787618-74-0P 787618-76-2P 787618-84-2P
787618-85-3P 787618-86-4P 787618-87-5P
787618-88-6P 787618-89-7P 787618-90-0P
787618-92-2P 787618-97-7P 787619-14-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of pyrazolopyrimidinones as PDE9 inhibitors for
treating type 2 diabetes, metabolic syndrome, and cardiovascular disease)
RN 787618-74-0 CAPLUS
CN L-Proline, 1-[[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

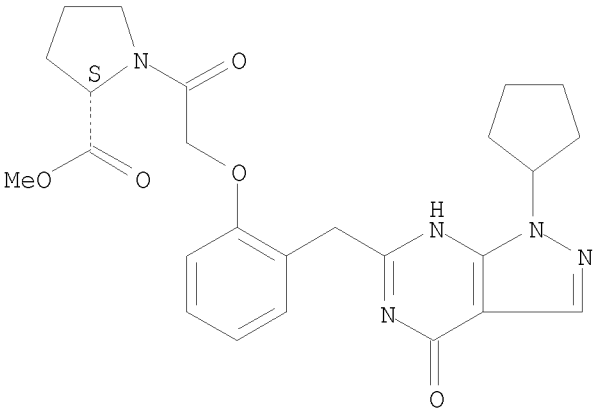


RN 787618-76-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-oxo-2-(1-piperazinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)

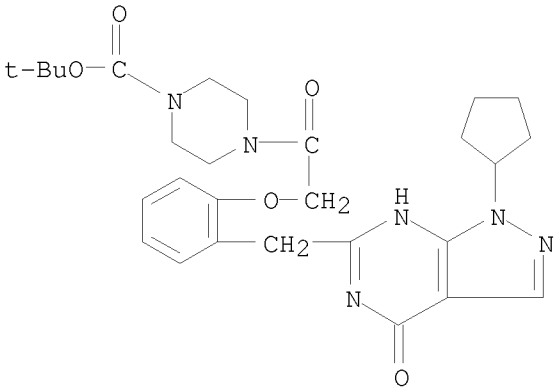


RN 787618-84-2 CAPLUS
CN L-Proline, 1-[[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

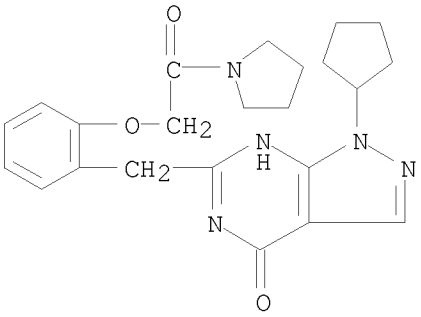
Absolute stereochemistry.



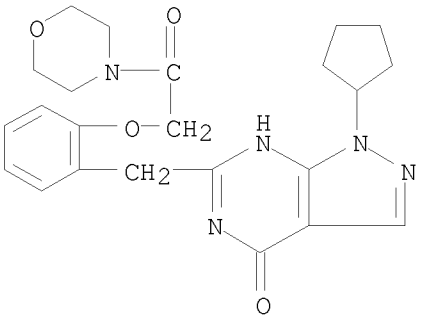
RN 787618-85-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



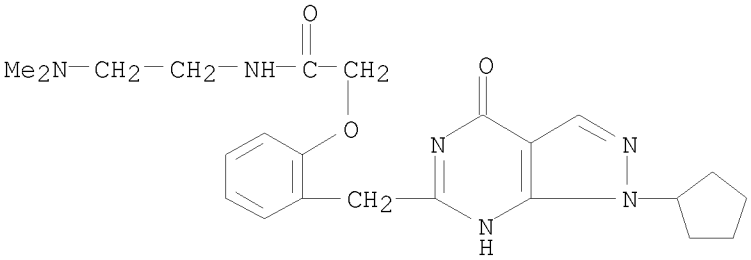
RN 787618-86-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-oxo-2-(1-pyrrolidinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)



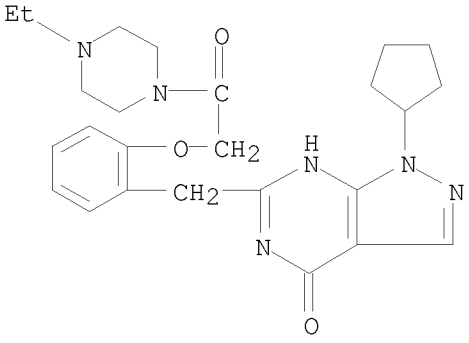
RN 787618-87-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)-2-oxoethoxy]phenyl]methyl]- (CA INDEX NAME)



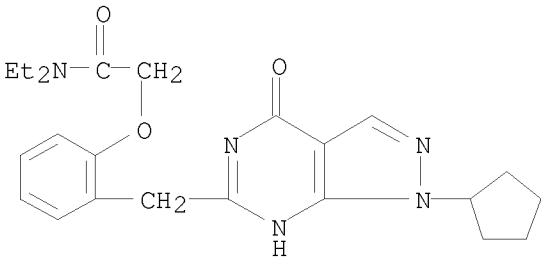
RN 787618-88-6 CAPLUS
CN Acetamide, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]-N-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



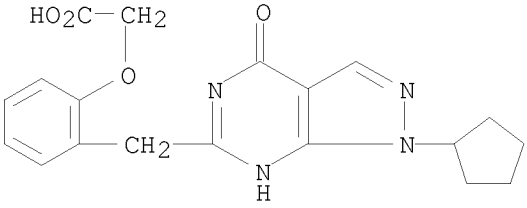
RN 787618-89-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[2-[2-(4-ethyl-1-piperazinyl)-2-oxoethoxy]phenyl]methyl]-1,5-dihydro- (CA INDEX NAME)



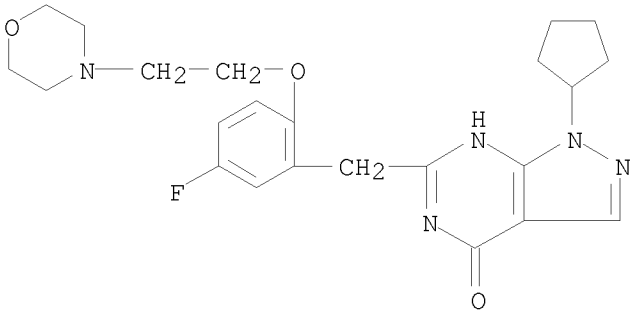
RN 787618-90-0 CAPLUS
CN Acetamide, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]-N,N-diethyl- (CA INDEX NAME)



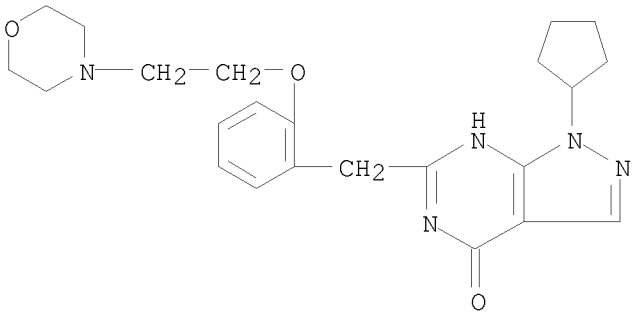
RN 787618-92-2 CAPLUS
CN Acetic acid, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]- (CA INDEX NAME)



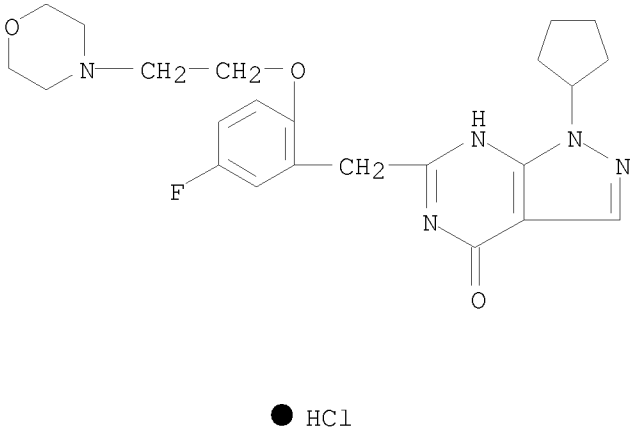
RN 787618-97-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[5-fluoro-2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-1,5-dihydro- (CA INDEX NAME)



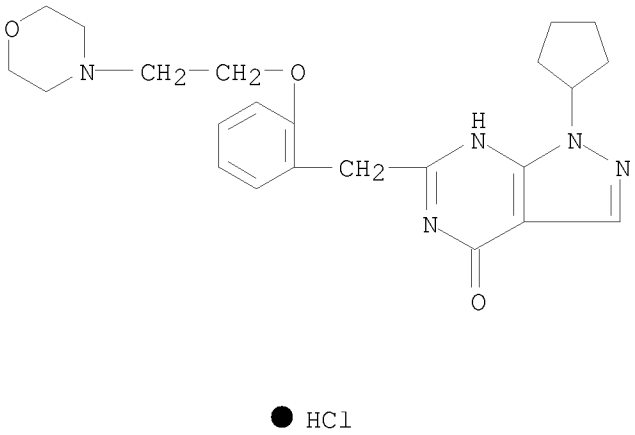
RN 787619-14-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)



IT 787619-25-4P 787619-37-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as PDE9 inhibitors for treating type 2 diabetes, metabolic syndrome, and cardiovascular disease)
RN 787619-25-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[5-fluoro-2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-1,5-dihydro-, hydrochloride (1:1) (CA INDEX NAME)

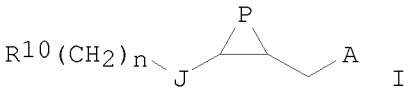


RN 787619-37-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

GI



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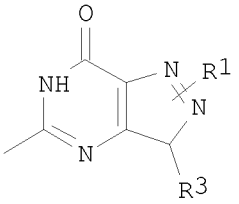
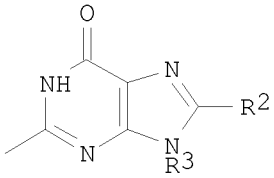
Q1 = 

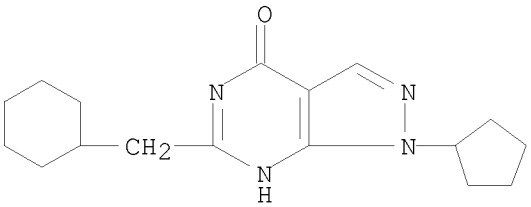
Q2 = 

AB Title compds. [I; A = Q1, Q2, etc.; P = atoms to form (substituted) cycloalkyl, heterocycloalkyl, aryl, heteroaryl rings; J = O, S, NR15, NR15CO, NR15SO2; R10 = CO2H, CONR30R31, NR15SO2R40; R1, R2, R15 = H, alkyl; R3 = alkyl, cycloalkyl, cycloalkylmethyl, heterocycloalkyl, heterocycloalkylmethyl, aryl, heteroaryl; R30, R31 = H, (substituted) alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; R30R31N = (substituted) 5-8 membered heterocyclyl; R40 = H, alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; n = 1-3], were prepared Thus, Et 1-[[2-(3-isopropyl-7-oxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-ylmethyl)phenoxy]acetyl]pyrrolidine-2-carboxylate was heated with aqueous NaOH in MeOH for 2 h at 58° to give after acidification with HCl 1-[[2-(3-isopropyl-7-oxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-ylmethyl)phenoxy]acetyl]pyrrolidine-2-carboxylic acid. Some compds. inhibited PDE9 with IC50 <50 nM.

L5 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:198173 CAPLUS
DOCUMENT NUMBER: 140:247085
TITLE: Selective phosphodiesterase 9A inhibitors for the improvement of cognitive processes
INVENTOR(S): Boss, Frank-Gerhard; Erb, Christina; Hendrix, Martin; Van Kampen, Marja; Wunder, Frank
PATENT ASSIGNEE(S): Bayer AG, Germany
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238722	A1	20040311	DE 2002-10238722	20020823
CA 2496292	A1	20040401	CA 2003-2496292	20030811
WO 2004026286	A2	20040401	WO 2003-EP8880	20030811
WO 2004026286	A3	20040603		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003258597	A1	20040408	AU 2003-258597	20030811
EP 1534285	A2	20050601	EP 2003-797233	20030811
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006501272	T	20060112	JP 2004-536933	20030811
US 20060100222	A1	20060511	US 2005-525119	20051014
PRIORITY APPLN. INFO.:			DE 2002-10238722 A	20020823
			WO 2003-EP8880 W	20030811

IT 667400-78-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phosphodiesterase 9A inhibitors for improvement of cognitive processes)
RN 667400-78-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)

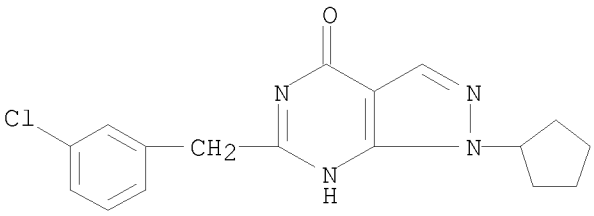


AB The invention discloses the use of selective phosphodiesterase 9A inhibitors for the production of drugs for the improvement of perception, concentration, cognitive processes, learning and/or memory. Preparation and activity of pyrazolopyrimidinone derivs. is included.

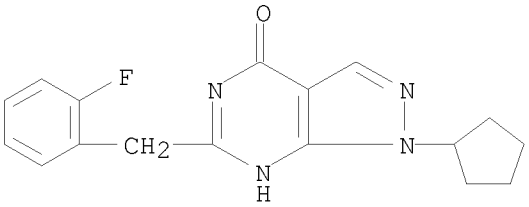
L5 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:182883 CAPLUS
DOCUMENT NUMBER: 140:217660
TITLE: Preparation of 6-benzylpyrazolo[3,4-d]pyrimidin-4-ones as phosphodiesterase-9A (PDE9A) inhibitors.
INVENTOR(S): Hendrix, Martin; Boess, Frank-Gerhard; Burkhardt, Nils; Erb, Christina; Tersteegen, Adrian; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018474	A1	20040304	WO 2003-EP8923	20030812
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10238723	A1	20040311	DE 2002-10238723	20020823
CA 2496194	A1	20040304	CA 2003-2496194	20030812
AU 2003258601	A1	20040311	AU 2003-258601	20030812
EP 1534711	A1	20050601	EP 2003-792301	20030812
EP 1534711	B1	20060419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006507242	T	20060302	JP 2004-530129	20030812
ES 2263057	T3	20061201	ES 2003-792301	20030812
US 20060106035	A1	20060518	US 2005-525115	20050831
PRIORITY APPLN. INFO.:			DE 2002-10238723 A	20020823
			WO 2003-EP8923 W	20030812

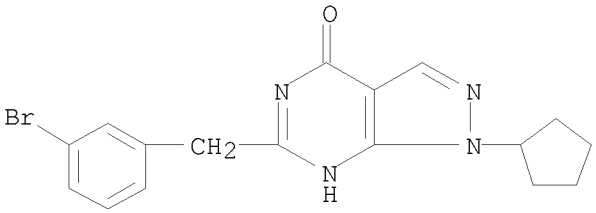
OTHER SOURCE(S): MARPAT 140:217660
IT 666235-19-4P 666235-20-7P 666235-21-8P
666235-22-9P 666235-23-0P 666235-24-1P
666235-26-3P 666235-30-9P 666235-32-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzylpyrazolopyrimidones as phosphodiesterase-9A (PDE9A) inhibitors)
RN 666235-19-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



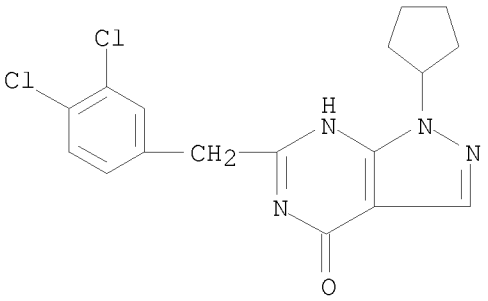
RN 666235-20-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[(2-fluorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



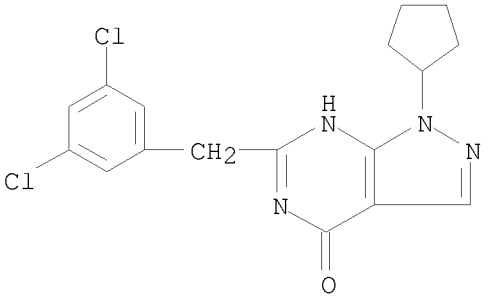
RN 666235-21-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-bromophenyl)methyl]-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



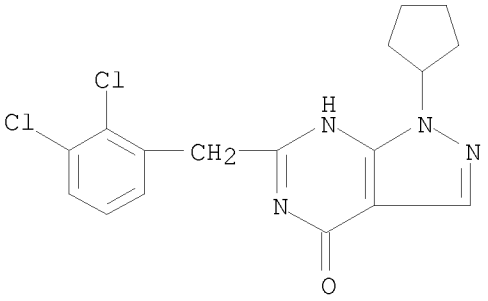
RN 666235-22-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



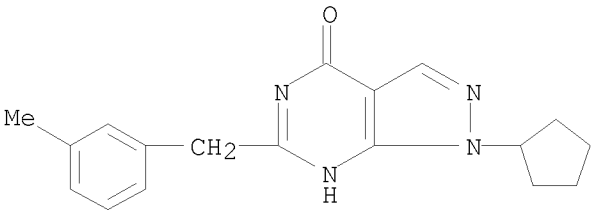
RN 666235-23-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[(3,5-dichlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



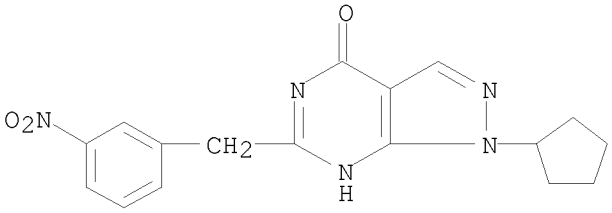
RN 666235-24-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[(2,3-dichlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



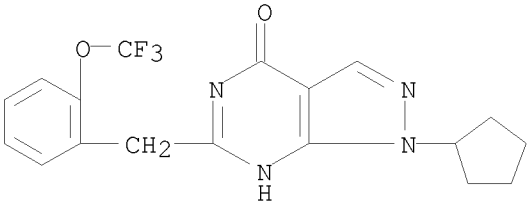
RN 666235-26-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(3-methylphenyl)methyl]- (CA INDEX NAME)



RN 666235-30-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(3-nitrophenyl)methyl]- (CA INDEX NAME)



RN 666235-32-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



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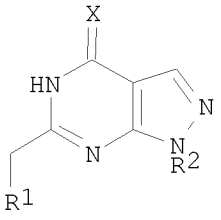


I

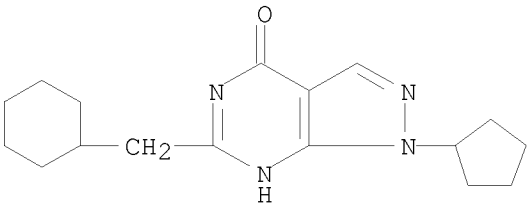
AB Title compds. (I; R1 = Ph substituted by 1-5 halo, alkyl, CF3, OCF3, cyano, OH, NO2, alkoxy; R2 = pentan-3-yl, C4-6 cycloalkyl; X = O, S), were prepared for improvement of perception, concentration, learning and/or memory (no data). Thus, 5-amino-1-cyclopentyl-1H-pyrazole-4-carboxamide (preparation given) and Et 3-chlorophenylacetate in EtOH at 0° were treated slowly with NaH followed by slow warming and then 18 h reflux to give 81% 6-(3-chlorobenzyl)-1-cyclopentyl-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

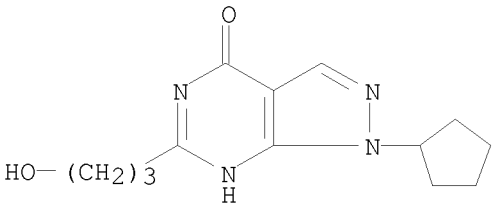
L5 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:177919 CAPLUS
DOCUMENT NUMBER: 140:235735
TITLE: Preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.
INVENTOR(S): Hendrix, Martin; Boess, Frank-Gerhard; Burkhardt, Nils; Erb, Christina; Tersteegen, Adrian; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238724	A1	20040304	DE 2002-10238724	20020823
CA 2496308	A1	20040401	CA 2003-2496308	20030813
WO 2004026876	A1	20040401	WO 2003-EP8979	20030813
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003251706	A1	20040408	AU 2003-251706	20030813
EP 1534713	A1	20050601	EP 2003-797239	20030813
EP 1534713	B1	20060111		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503051	T	20060126	JP 2004-536941	20030813
ES 2256797	T3	20060716	ES 2003-797239	20030813
US 20060111372	A1	20060525	US 2005-524956	20051215
PRIORITY APPLN. INFO.:			DE 2002-10238724 A	20020823
			WO 2003-EP8979 W	20030813

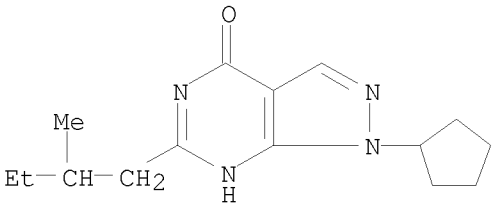
OTHER SOURCE(S): MARPAT 140:235735
IT 667400-78-4P 667870-10-2P 667870-11-3P
667870-12-4P 667870-13-5P 667870-22-6P
667870-24-8P 667870-25-9P 667870-27-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)
RN 667400-78-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



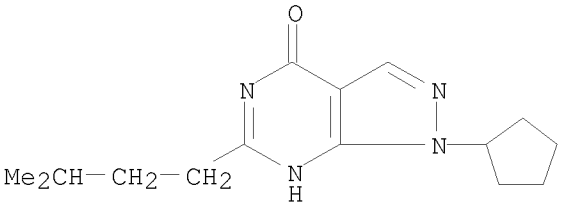
RN 667870-10-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(3-hydroxypropyl)- (CA INDEX NAME)



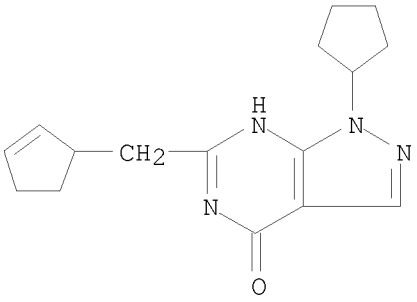
RN 667870-11-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(2-methylbutyl)- (CA INDEX NAME)



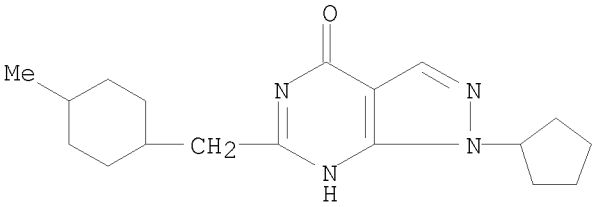
RN 667870-12-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(3-methylbutyl)- (CA INDEX NAME)



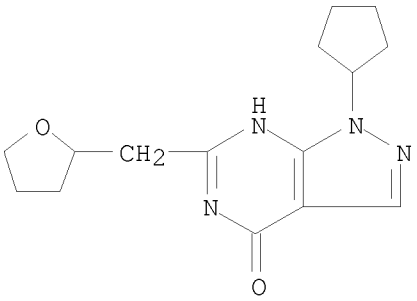
RN 667870-13-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



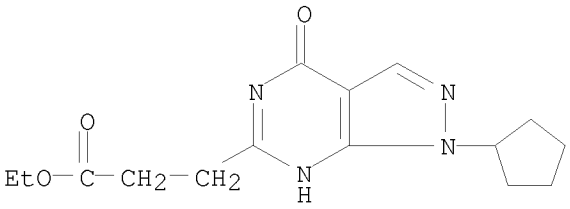
RN 667870-22-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(4-methylcyclohexyl)methyl]- (CA INDEX NAME)



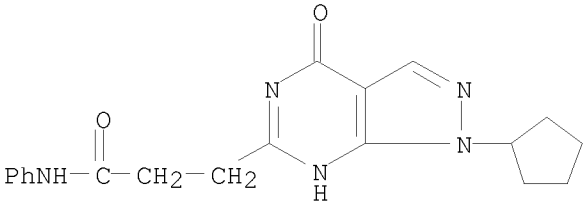
RN 667870-24-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)



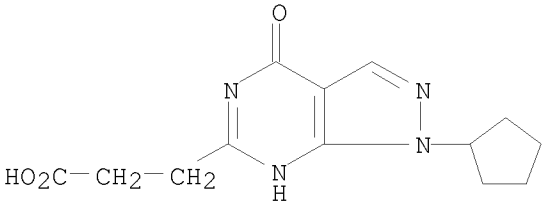
RN 667870-25-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-cyclopentyl-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)



RN 667870-27-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanamide, 1-cyclopentyl-4,5-dihydro-4-oxo-N-phenyl- (CA INDEX NAME)



IT 667870-31-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)
RN 667870-31-7 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-cyclopentyl-4,5-dihydro-4-oxo- (CA INDEX NAME)



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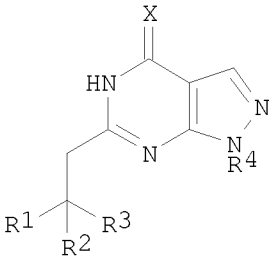


I

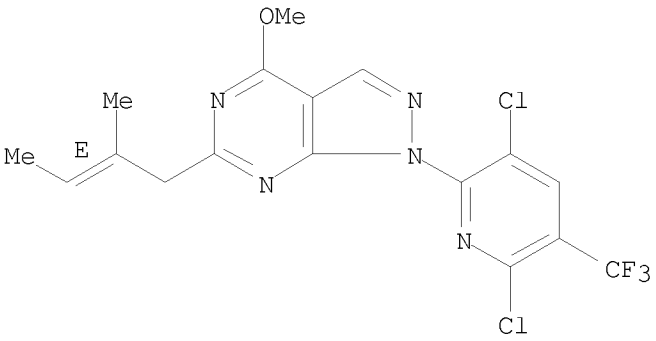
AB Title compds. [I; R1 = OH, (substituted) alkyl, alkoxy, CO2R5, CONR6R7; R5 = alkyl; R6, R7 = H, aryl, alkyl; NR6R7 = 4-10 membered heterocycle; R2 = H, alkyl, alkoxy; R3 = H, alkyl; R4 = pentan-3-yl, C4-6 cycloalkyl; X = O, S], were prepared Thus, 5-amino-1-cyclopentyl-1H-pyrazole-4-carboxamide (preparation given), Me cyclohexylacetate, and NaH were refluxed 18 h in EtOH to give 31% 6-cyclohexylmethyl-1-cyclopentyl-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

L5 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:891929 CAPLUS
DOCUMENT NUMBER: 139:381500
TITLE: Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides
INVENTOR(S): Linker, Karl-Heinz; Andree, Roland; Hoischen, Dorothee; Schwarz, Hans-Georg; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter
PATENT ASSIGNEE(S): Bayer CropScience AG, Germany
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

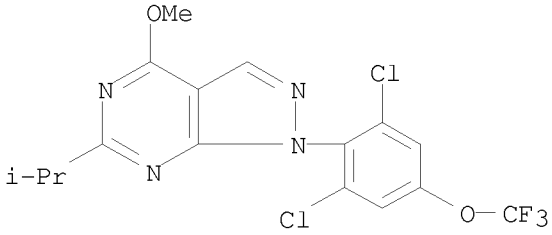
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10219435	A1	20031113	DE 2002-10219435	20020502
IN 2003MU00379	A	20050211	IN 2003-MU379	20030417
CA 2484997	A1	20031113	CA 2003-2484997	20030422
WO 2003093269	A2	20031113	WO 2003-EP4137	20030422
WO 2003093269	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003224111	A1	20031117	AU 2003-224111	20030422
EP 1504005	A2	20050209	EP 2003-720510	20030422
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009873	A	20050426	BR 2003-9873	20030422
JP 2005531549	T	20051020	JP 2004-501408	20030422
US 20050209251	A1	20050922	US 2005-512834	20050519
PRIORITY APPLN. INFO.:			DE 2002-10219435 A	20020502
			WO 2003-EP4137 W	20030422

OTHER SOURCE(S): MARPAT 139:381500
IT 1053783-27-9 1053783-28-0 1053783-32-6
1053783-35-9 1053783-56-4 1053783-57-5
1053783-58-6 1053783-61-1 1053783-62-2
1053783-64-4 1053783-68-8 1053783-73-5
1053783-77-9 1053783-82-6 1053783-83-7
1053783-90-6 1053783-93-9 1053783-95-1
1053783-96-2 1053783-99-5 1053784-26-1
RL: PRPH (Prophetic)
(Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides)
RN 1053783-27-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

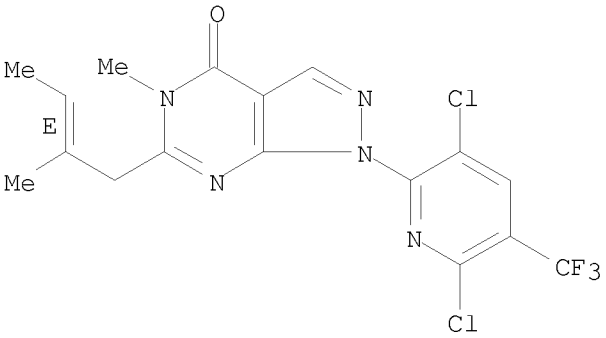


RN 1053783-28-0 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

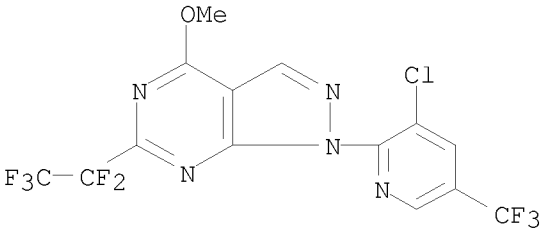


RN 1053783-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

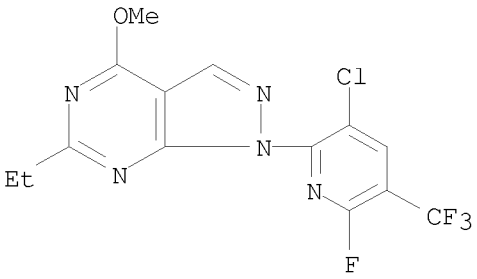
Double bond geometry as shown.



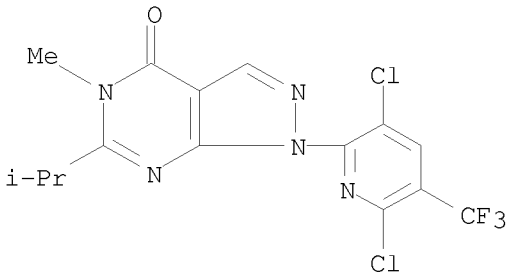
RN 1053783-35-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(1,1,2,2,2-pentafluoroethyl)- (CA INDEX NAME)



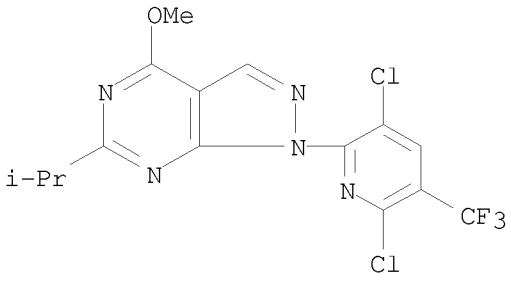
RN 1053783-56-4 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-6-fluoro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-4-methoxy- (CA INDEX NAME)



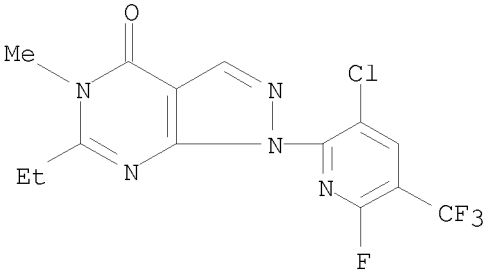
RN 1053783-57-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



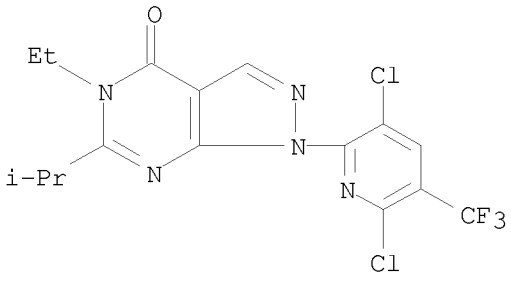
RN 1053783-58-6 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



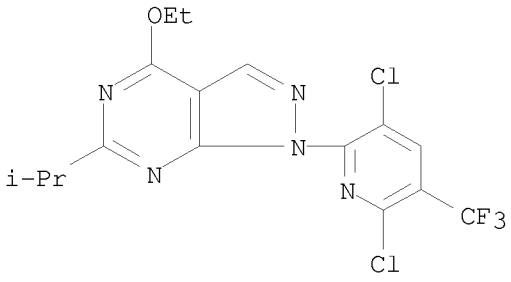
RN 1053783-61-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-6-fluoro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro-5-methyl- (CA INDEX NAME)



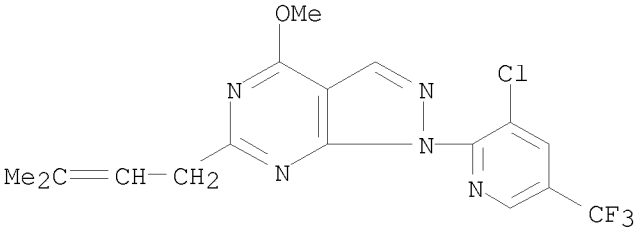
RN 1053783-62-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-5-ethyl-1,5-dihydro-6-(1-methylethyl)- (CA INDEX NAME)



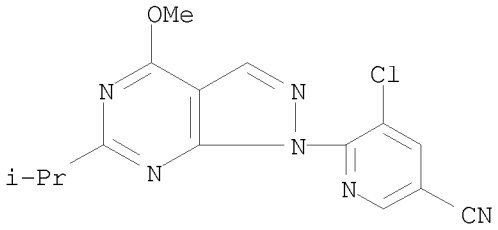
RN 1053783-64-4 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-ethoxy-6-(1-methylethyl)- (CA INDEX NAME)



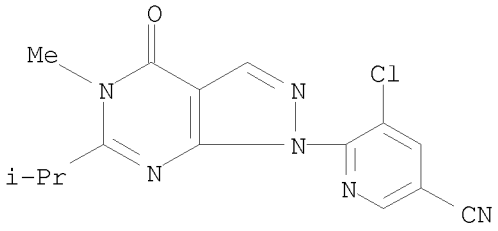
RN 1053783-68-8 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(3-methyl-2-buten-1-yl)- (CA INDEX NAME)



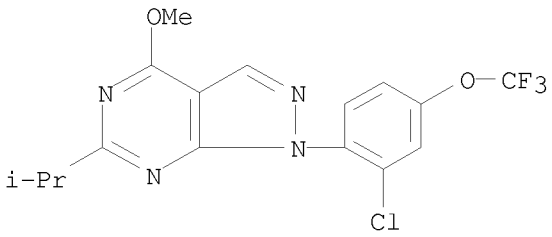
RN 1053783-73-5 CAPLUS
CN 3-Pyridinecarbonitrile, 5-chloro-6-[4-methoxy-6-(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



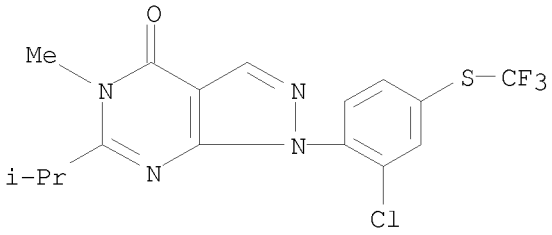
RN 1053783-77-9 CAPLUS
CN 3-Pyridinecarbonitrile, 5-chloro-6-[4,5-dihydro-5-methyl-6-(1-methylethyl)-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



RN 1053783-82-6 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2-chloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

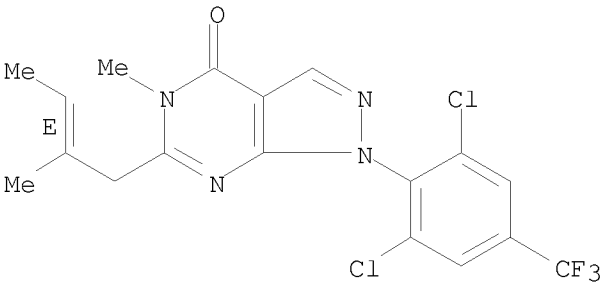


RN 1053783-83-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-[(trifluoromethyl)thio]phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

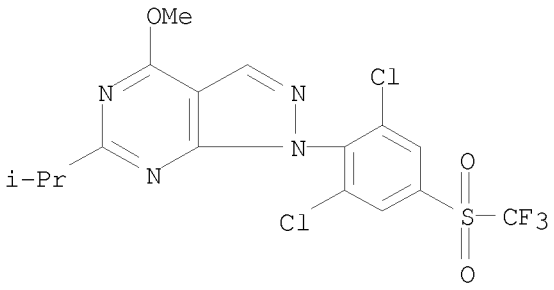


RN 1053783-90-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

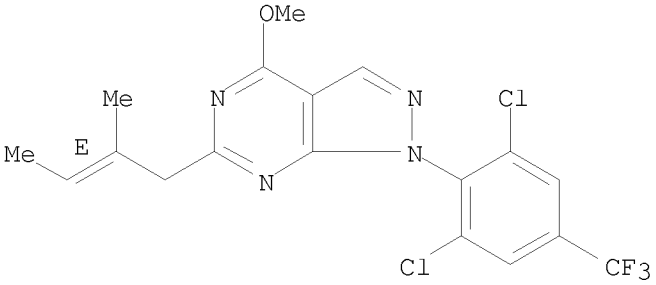


RN 1053783-93-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

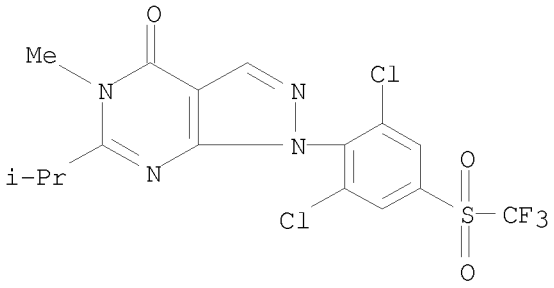


RN 1053783-95-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-methoxy-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

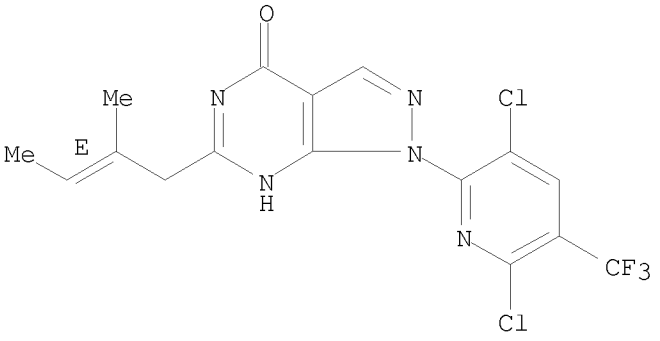


RN 1053783-96-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

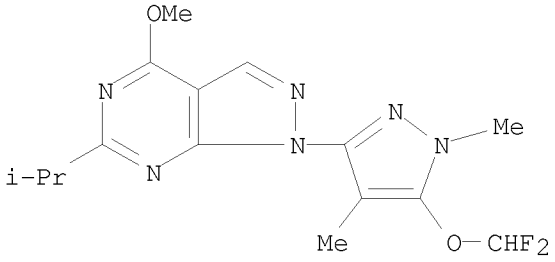


RN 1053783-99-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

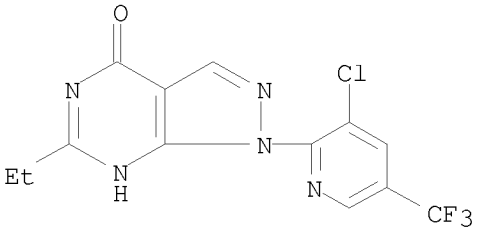
Double bond geometry as shown.



RN 1053784-26-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[5-(difluoromethoxy)-1,4-dimethyl-1H-pyrazol-3-yl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

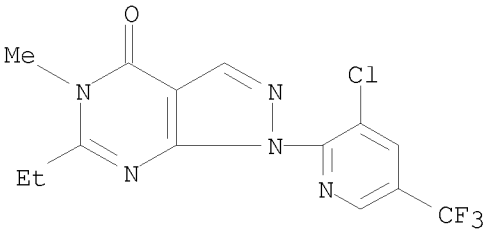


IT 623584-59-8P 623584-60-1P 623584-61-2P
623584-62-3P 623584-63-4P 623584-64-5P
623584-65-6P 623584-66-7P 623584-67-8P
623584-68-9P 623584-69-0P 623584-70-3P
623584-71-4P 623584-72-5P 623584-78-1P
623584-98-5P 623584-99-6P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as herbicides and/or nematocides)
RN 623584-59-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro- (CA INDEX NAME)

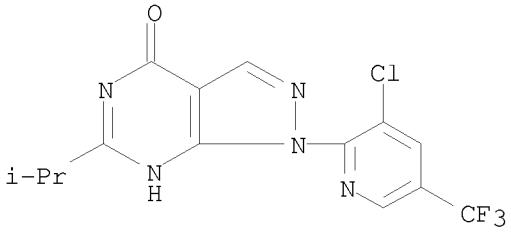


RN 623584-60-1 CAPLUS

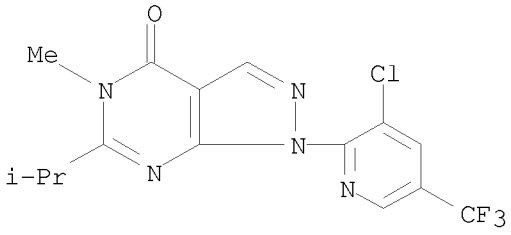
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro-5-methyl- (CA INDEX NAME)



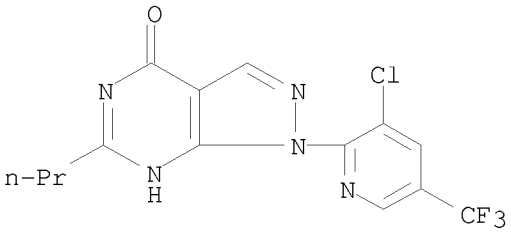
RN 623584-61-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(1-methylethyl)- (CA INDEX NAME)



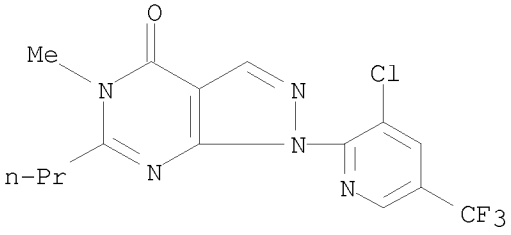
RN 623584-62-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



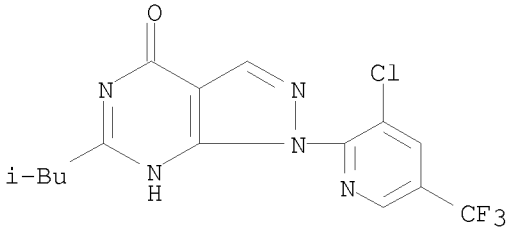
RN 623584-63-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-propyl- (CA INDEX NAME)



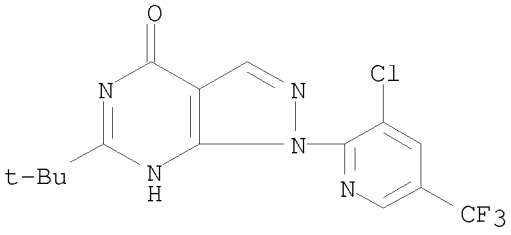
RN 623584-64-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-propyl- (CA INDEX NAME)



RN 623584-65-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(2-methylpropyl)- (CA INDEX NAME)

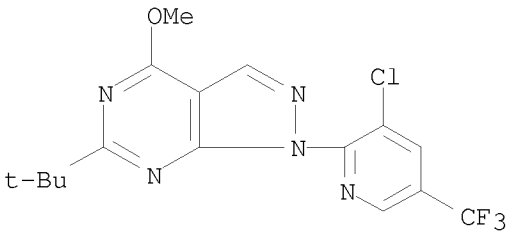


RN 623584-66-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-(1,1-dimethylethyl)-1,5-dihydro- (CA INDEX NAME)

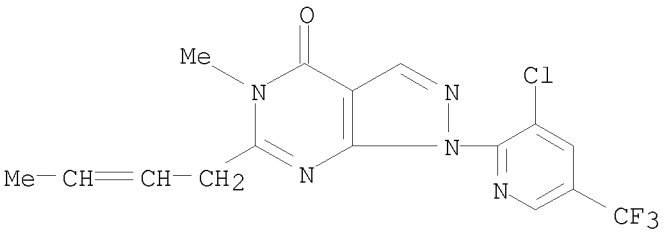


RN 623584-67-8 CAPLUS

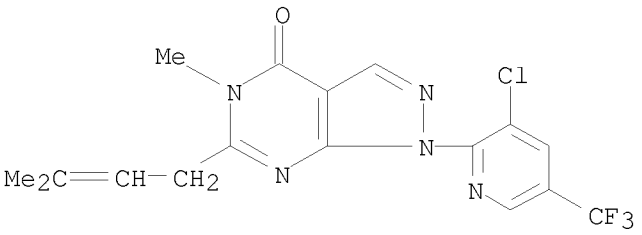
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



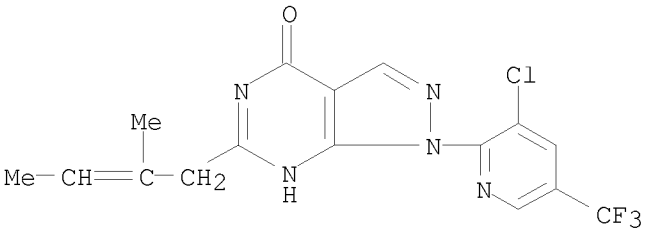
RN 623584-68-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-buten-1-yl)-1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl- (CA INDEX NAME)



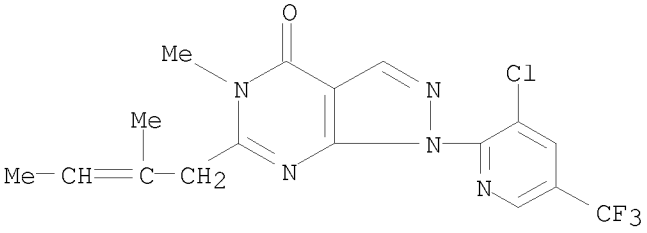
RN 623584-69-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(3-methyl-2-buten-1-yl)- (CA INDEX NAME)



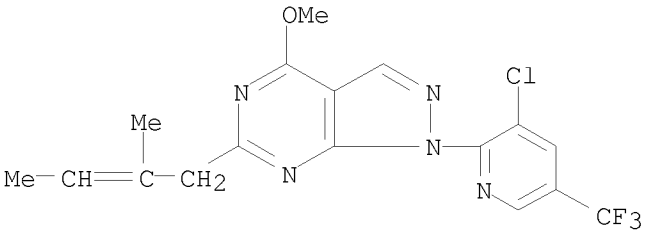
RN 623584-70-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)



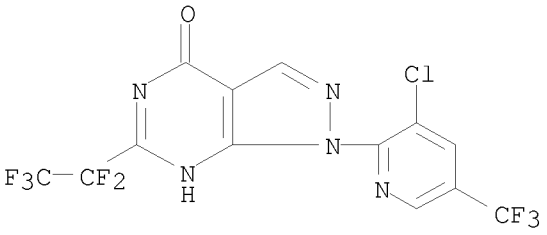
RN 623584-71-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)



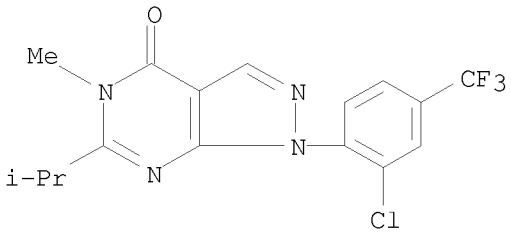
RN 623584-72-5 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)



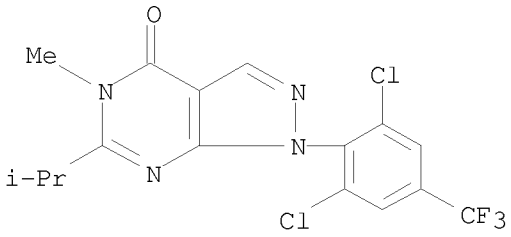
RN 623584-78-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(1,1,2,2,2-pentafluoroethyl)- (CA INDEX NAME)



RN 623584-98-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



RN 623584-99-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



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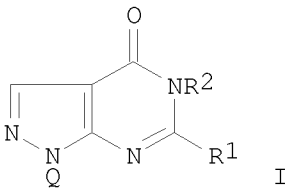
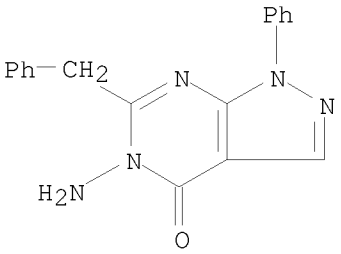


I

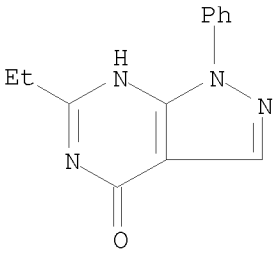
AB Title compds. [I; Q = NO2, cyano, halo, (halogenated) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, (hetero)aryl; R1 = H, (substituted) alkyl, alkoxycarbonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, heterocyclyl; R2 = H, (substituted) alkyl, alkenyl, alkynyl], were prepared Thus, a mixture of 5-amino-1-(3-chloro-5-trifluoromethylpyridin-2-yl)pyrazole-4-carboxamide, CH(OMe)3, p-toluenesulfonic acid, and toluene was refluxed for 12 h followed by further addition of CH(OMe)3 and reflux for 12 h under stirring to give 44% 1-(3-chloro-5-trifluoromethylpyridin-2-yl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one. I were said to show very strong pre- and postemergent herbicidal activity, good crop tolerance, and good nematocidal activity.

L5 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:736859 CAPLUS
DOCUMENT NUMBER: 140:163756
TITLE: Design, synthesis, and antimicrobial activity of some new pyrazolo[3,4-d]pyrimidines
AUTHOR(S): Abdel-Gawad, Soad M.; Ghorab, M. M.; El-Sharief, A. M. Sh.; El-Telbany, F. A.; Abdel-Alla, M.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science (Girl's), Al-Azhar University, Cairo, Egypt
SOURCE: Heteroatom Chemistry (2003), 14(6), 530-534
CODEN: HETCE8; ISSN: 1042-7163
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:163756
IT 654069-43-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis, and antibacterial activity of some new pyrazolo[3,4-d]pyrimidines from a phenylpyrazole carboxylate)
RN 654069-43-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

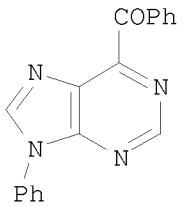


AB 2-Benzyl- and 2-aryloxymethyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidine-4-ones were synthesized by reacting arylacetylamino derivs. with hydrazine hydrate. Thionation of the above compds. by action of P2S5 in pyridine yielded 2-aryloxy-methyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidin-4-thiones. 2,5-Diphenyl-2,3-dihydro-1H-pyrazolo[5',1':4:5]-pyrazolo[3,4-d]pyrimidine-8-one was also obtained via reaction of ethyl-2-cinnamoylamino-1-phenyl-pyrazole-4-car-boxylate with hydrazine hydrate. The prepared compds. were screened in vitro for their antimicrobial activity. Some of the tested compds. were found to be active at 100 μg/mL compared with reference compds. (Ampicillin and Trivid) as antibacterial agents and claforan as antifungal agent.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:226504 CAPLUS
DOCUMENT NUMBER: 128:282737
ORIGINAL REFERENCE NO.: 128:55970h,55971a
TITLE: Catalytic action of azolium salts. IX. Synthesis of 6-aroyl-9H-purines and their analogs by nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt
AUTHOR(S): Miyashita, Akira; Suzuki, Yumiko; Iwamoto, Ken-Ichi; Higashino, Takeo
CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, 422, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(3), 390-399
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:282737
IT 5394-42-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 6-aroyl-9H-purines and analogs via nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



GI



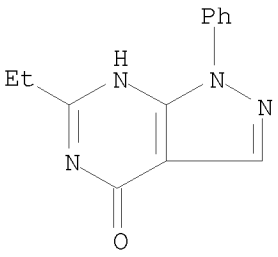
II

AB In the presence of 1,3-dimethylimidazolium iodide (I), 6-chloro-9-phenyl-9H-purine and 4-chloro-5,6-dimethylpyrrolo[2,3-d]pyrimidines underwent nucleophilic aroylation with arenecarbaldehydes to give the corresponding fused aroylpyrimidines, e.g. II. 1,3-Dimethylbenzimidazolium iodide (III) was an effective catalyst for the

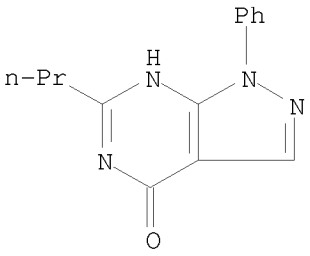
similar synthesis of 7-aroyl-3-phenyl-3H-1,2,3-triazolo[4,5-d]pyrimidines. In the synthesis of 4-aroyl-1H-pyrazolo[3,4-d]pyrimidines, both azolium salts I and III were effective as catalysts. Moreover, 4-aroyl-7H-pyrrolo[2,3-d]pyrimidines were obtained in good yields via the 4-tosyl derivs., in the presence of catalytic amts. of sodium p-toluenesulfinate and the imidazolium salt I. This catalytic aroylation was found to be a facile and useful method for the synthesis of 6-aroyl-9H-purines and their analogs.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

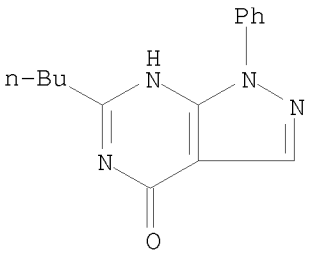
L5 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:174107 CAPLUS
DOCUMENT NUMBER: 116:174107
ORIGINAL REFERENCE NO.: 116:29471a,29474a
TITLE: Versatile synthesis of 6-alkyl(aryl)-1H-pyrazolo[3,4-d]pyrimidin-4[5H]-ones
AUTHOR(S): Reddy, K. Hemender; Reddy, A. Panduranga; Veeranagaiah, V.
CORPORATE SOURCE: Nizam Coll., Osmania Univ., Hyderabad, 500 001, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1992), 31B(3), 163-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:174107
IT 5394-42-3P 130925-64-3P 139954-52-2P
139954-53-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



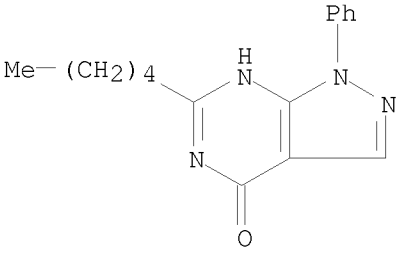
RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA INDEX NAME)



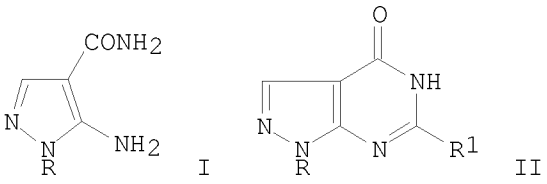
RN 139954-52-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-butyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 139954-53-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-pentyl-1-phenyl- (CA INDEX NAME)

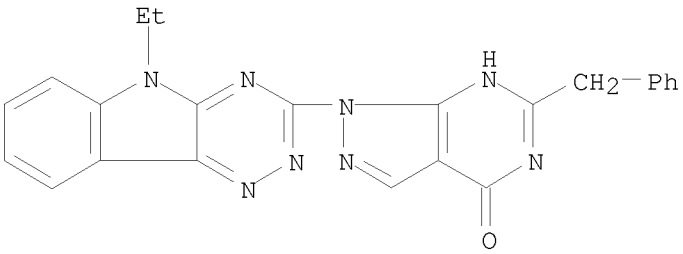


GI

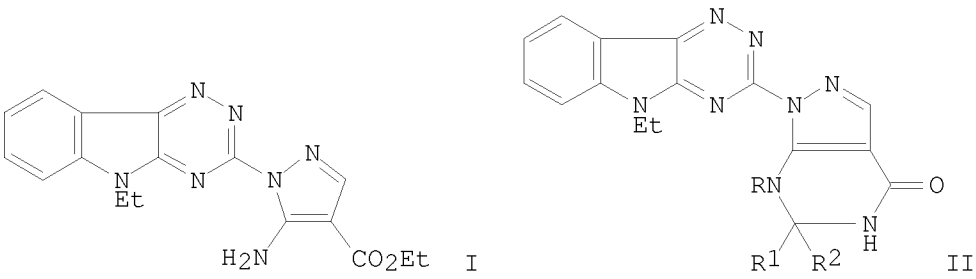


AB Condensation of 5-amino-1H-pyrazole-4-carboxamide (I, R = H) with various aromatic aldehydes furnishes 6-substituted 1H-pyrazole[3,4-d]pyrimidin-4(5H)-ones II (R1 = Ph, substituted Ph) via the intermediate 5-(N-arylideneamino)pyrazole-4-carboxamides. II were also synthesized by the reaction of I (R = H) with aromatic carboxylic acids in polyphosphoric acid (PPA) or polyphosphate ester (PPE). Similar treatment of I (R = Ph, Me) with aromatic aldehydes and aromatic carboxylic acids gives exclusively 6-substituted 1-methyl/phenyl-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones. The title compds. have were also synthesized by the reaction of I with arylideneanilines.

L5 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:429256 CAPLUS
DOCUMENT NUMBER: 115:29256
ORIGINAL REFERENCE NO.: 115:5149a,5152a
TITLE: Synthesis of ethyl-5-amino-1-(5-ethyl-5H-1,2,4-triazino[5,6-b]indol-3-yl)-1H-pyrazole-4-carboxylate and pyrazolo[3,4-d]pyrimidine derivatives
AUTHOR(S): Younes, M. I.; Abbas, H. H.; Metwally, S. A. M.
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Quena, Egypt
SOURCE: Pharmazie (1991), 46(2), 98-100
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 134513-78-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 134513-78-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(5-ethyl-5H-1,2,4-triazino[5,6-b]indol-3-yl)-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)

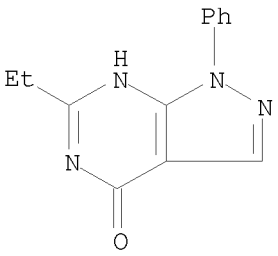


GI

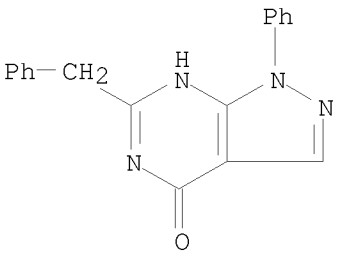


AB Ethoxymethylene cyanoacetate reacts with 5-ethyl-3-hydrazino-5H-1,2,4-trizino[5,6-b]indole to give amino(triazinoindolyl)pyrazolecarboxylate (I). I reacts with urea, thiourea and benzylnitrile to give pyrazolo[3,4-d]pyrimidine derivs. II (R = H, R1R2 = O, S; RR1 = bond, R2 = CH2Ph, resp.). The reaction of I with other reagents such as acid chlorides, acid anhydrides, hydrazines and ammonium thiocyanate was also studied.

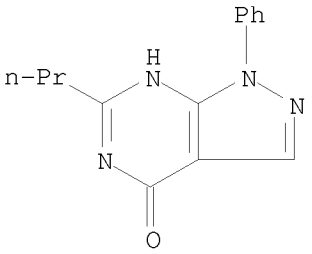
L5 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:6429 CAPLUS
DOCUMENT NUMBER: 114:6429
ORIGINAL REFERENCE NO.: 114:1267a,1270a
TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. XVIII. Facile preparation of 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones
AUTHOR(S): Miyashita, Akira; Iijima, Chihoko; Higashino, Takeo; Matsuda, Hideaki
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SOURCE: Heterocycles (1990), 31(7), 1309-14
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:6429
IT 5394-42-3P 94331-62-1P 130925-64-3P
130925-65-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



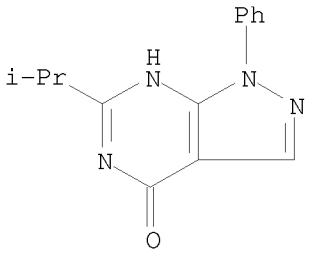
RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



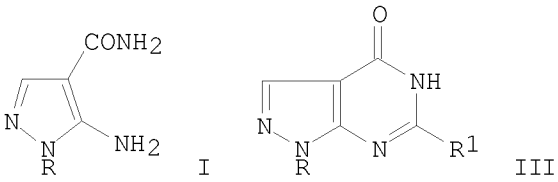
RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA INDEX NAME)



RN 130925-65-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(1-methylethyl)-1-phenyl- (CA INDEX NAME)

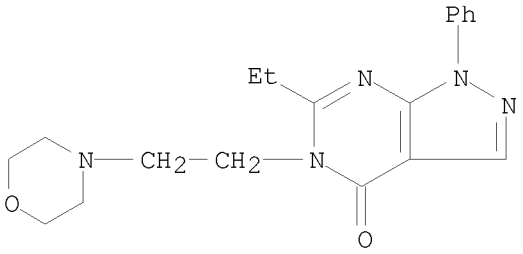


GI

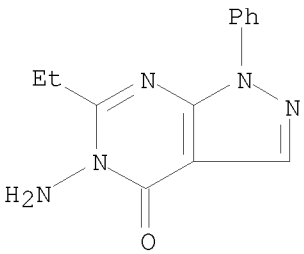


AB Reaction of 5-amino-1-phenyl-1H-pyrazole-4-carboxamide (I, R = Ph) with R1CO2R2 (II, R1 = H, Me, Et, Pr, Me2CH, PHCH2, CO2Et, Ph; R2 = Me, Et) in the presence of EtONa-EtOH gave 1-phenylpyrazolopyrimidinones III (R = Ph). Similar treatment of I (R = Me) with II gave III (R = Me).

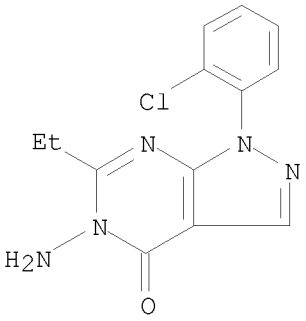
L5 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:567969 CAPLUS
DOCUMENT NUMBER: 87:167969
ORIGINAL REFERENCE NO.: 87:26547a,26550a
TITLE: Synthesis of condensed heterocyclic systems of pyrazole
AUTHOR(S): Alonso, G.; Madronero, R.; Nebreda, L.
CORPORATE SOURCE: Inst. Quim. Med., Madrid, Spain
SOURCE: Anales de Quimica (1968-1979) (1976), 72(11-12), 897-901
CODEN: ANQUBU; ISSN: 0365-4990
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
IT 64257-08-5P 64257-09-6P 64257-10-9P
64257-17-6P 64257-19-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64257-08-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-5-[2-(4-morpholinyl)ethyl]-1-phenyl- (CA INDEX NAME)



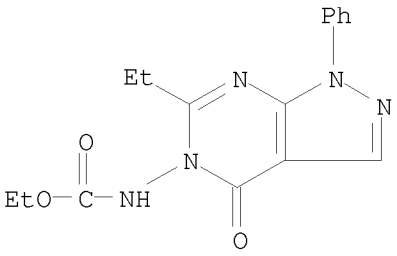
RN 64257-09-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



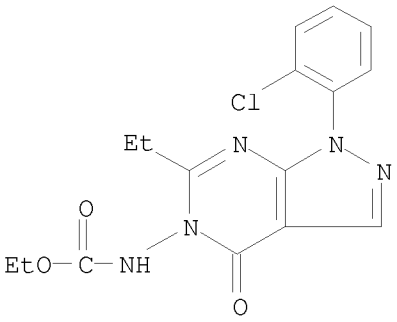
RN 64257-10-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-1-(2-chlorophenyl)-6-ethyl-1,5-dihydro- (CA INDEX NAME)



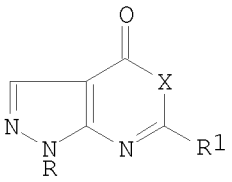
RN 64257-17-6 CAPLUS
CN Carbamic acid, (6-ethyl-1,4-dihydro-4-oxo-1-phenyl-5H-pyrazolo[3,4-d]pyrimidin-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)



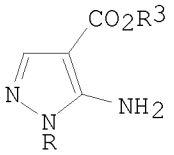
RN 64257-19-8 CAPLUS
CN Carbamic acid, [1-(2-chlorophenyl)-6-ethyl-1,4-dihydro-4-oxo-5H-pyrazolo[3,4-d]pyrimidin-5-yl]-, ethyl ester (9CI) (CA INDEX NAME)



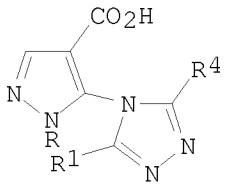
GI



I



II



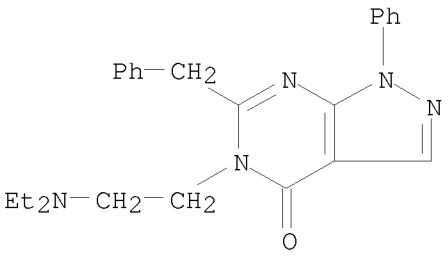
III

AB Pyrazolopyrimidines I (R = Ph, 2-ClC6H4; R1 = Me, Et; X = NR2, R2 = morpholinoethyl, morpholinopropyl, NH2, NHPh) were prepared by condensing EtOCH:C(CN)CO2Et with RNHNH2, hydrolyzing II (R3 = Et), cyclizing II (R3 = H) with (R1CO)2O, and treating I (X = O), with R2NH2. Reaction of I (X = O) with H2NNHCO2Et gave I (X = NNHCO2Et), whereas R4CONHNH2 (R4 = CHMe2, CH2CN, 2-furyl, 3-pyridiyl, 1-naphthyl, 2-naphthyl, 3-indolyl, 2-indolyl, Me, Ph, PhCH2) gave III and 1-naphthylacetylhydrazine gave a mixture of I (X = NNHCOCH2C10H7) and III (R4 = 1-naphthylmethyl).

L5 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:22609 CAPLUS
DOCUMENT NUMBER: 62:22609
ORIGINAL REFERENCE NO.: 62:4037c-e
TITLE: Pyrazolo[3,4-d]pyrimidines
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

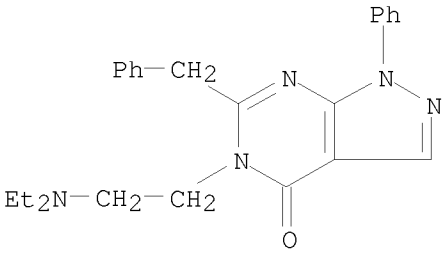
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 973361		19641028	GB 1961-17103	19610510
PRIORITY APPLN. INFO.:			CH	19600511

IT 1177-04-4
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1177-04-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, monohydrochloride (8CI) (CA INDEX NAME)

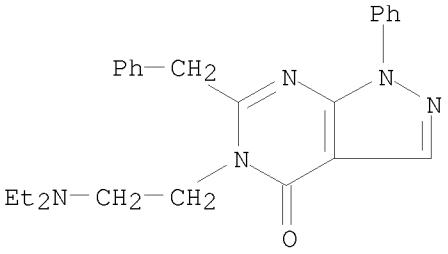


● HCl

IT 1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-
101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 1254-49-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl- (7CI, 8CI) (CA INDEX NAME)



RN 101405-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-, hydrochloride (1:?) (CA INDEX NAME)

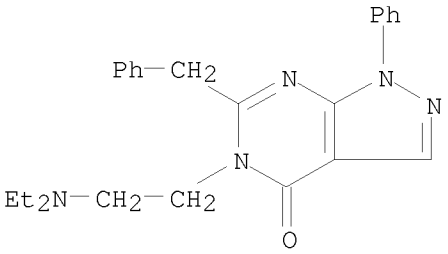


GI For diagram(s), see printed CA Issue.
AB The title compds. (I) were prepared by alkylating a 1,6-disubstituted 4-hydroxypyrazolo[3,4-d]pyrimidine with a dialkylaminoalkyl chloride or Me2SO4. Thus, a solution of 1.15 g. Na in 40 ml. EtOH was added to 14.1 g. 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine followed by 7.5 g. Et2NCH2CH2Cl and the mixture refluxed 4 hrs. to give the hydrochloride of I (R1 = sec-Bu, R2 = Et2NCH2CH2, R3 = PhCH2), m. 147-8°. The following I were prepared similarly (R1, R2, R3, m.p. free base, and m.p. hydrochloride given): iso-Pr, Me, PhCH2, 96-7°, --; iso-Pr, Me2NCH2CH2, PhCH2, 115-17°, 229-31°; iso-Pr, Et2NCH2CH2, PhCH2, --, 202-3°; iso-Pr, Et2N(CH2)3, PhCH2, 70-1°, 173-5°; Me, Et2NCH2CH2, PhCH2, 83-5°, 219°; Ph, Et2NCH2CH2, PhCH2, 103-5°, 225°; iso-Pr, Et2NCH2CH2, Me, --, --; iso-Pr, Me, iso-Pr, 75-7°, --; iso-Pr, Et2NCH2CH2, iso-Pr, --(b0.05 138-40°), --; iso-Pr, Et2NCH2CH2, Ph2CH, 124-5°, --. The title compds. had coronary dilating properties.

L5 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:22608 CAPLUS
DOCUMENT NUMBER: 62:22608
ORIGINAL REFERENCE NO.: 62:4037a-c
TITLE: O-(α-Tetrahydropyranyl)-S-alkoxycarbonyl thiamines with vitamin B1 activity
INVENTOR(S): Takamizawa, Akira; Hirai, Kentaro
PATENT ASSIGNEE(S): Shionogi & Co., Ltd.
SOURCE: 17 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR M2755		19640928	FR	
DE 1226586			DE	
PRIORITY APPLN. INFO.:			JP	19620727

OTHER SOURCE(S): MARPAT 62:22608
IT 1177-04-4
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1177-04-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

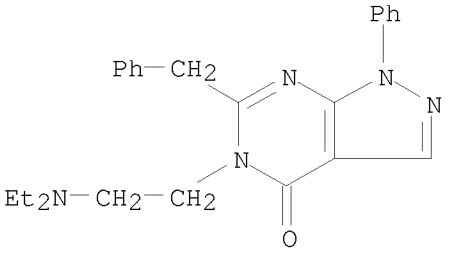
GI For diagram(s), see printed CA Issue.
AB I (R = 2-pyranyl) have a rapid and long-lasting vitamin B1 activity. They are prepared by the reaction of I (R = H, II) with 4H-dihydropyran in the presence of an acid catalyst. II are prepared from the alkali salts III (where M = Na or K) of the thiol form of thiamine (IV) with compds. XCOYR, where X is a halogen atom. Thus, 0.35 mL. HCl is added to a suspension of 1 g. S-ethoxycarbonylthiamine (V) in 10 mt. 4H-dihydropyran, the mixture stirred, the separated crystals are taken up in H2O, the solution is shaken with Et2O, and NH4OH added to precipitate 0.80 g. O-(α-tetrahydropyranyl)-S-(ethoxycarbonyl)thiamine, m. 73-4° (H2O + EtOH). For the preparation of V, m. 140° (decomposition) (AcOEt), IV.HCl is dissolved in aqueous NaOH, the solution saturated with NaCl, and ClCO2Et added. Other compds. prepared are O-(α-tetrahydropyranyl)-S-(butoxycarbonyl)thiamine, m. 125°; S-butoxycarbonylthiamine, m. 139-40° (decomposition);

O-(α-tetrahydropyranyl)-S-ethylthiocarbonylthiamine, m. 102-3°; and S-ethylthiocarbonylthiamine, m. 136-7° (decomposition).

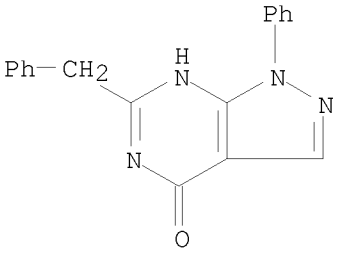
L5 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:469189 CAPLUS
DOCUMENT NUMBER: 59:69189
ORIGINAL REFERENCE NO.: 59:12820a-h,12821a
TITLE: Pyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1149013		19630522	DE	
PRIORITY APPLN. INFO.:			CH	19600511

IT 1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl- 94331-62-1P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-phenyl- 101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 1254-49-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl- (7CI, 8CI) (CA INDEX NAME)

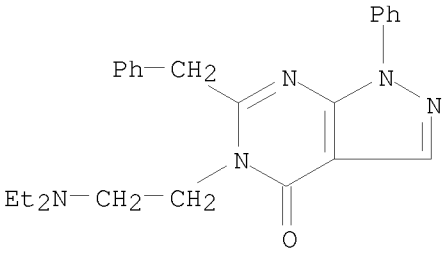


RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



RN 101405-08-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-, hydrochloride (1:?) (CA INDEX NAME)



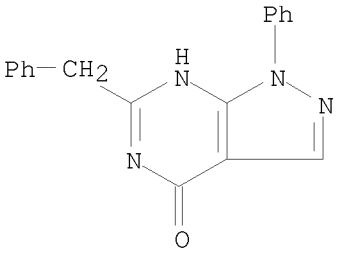
●x HCl

GI For diagram(s), see printed CA Issue.

AB 4-Oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (I), possessing vasodilating ability, are described in which R1 = H, alkyl or phenyl group, R2 = H or lower alkyl group, R3 = HO, halogen, NR5R6 (R5 and R6 = H, alkyl groups or joined together through O, S, or N) (or the position may be unsubstituted), R4 = alkyl or aralkyl group. The most active compds., I (R1 = iso-Pr, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (II) and I (R1 = sec-Bu, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (III) at a concentration of 10 γ/ml. increase coronary blood flow 78-73% in the Langendorf isolated dog heart procedure. In the same test, 1-isopropyl-4-diethylaminopyrazolo-[3,4-d]pyrimidine (CA 55, 13457a) at the same concentration causes an increase of 60%. In the compds. described below R2 = H. Na (2.3 g.) is finely dispersed in 50 ml. PhCH2CN and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole (IV) added. The mixture is heated to 110-20° with stirring for 4 hrs. and cooled, 100 ml. alc. is added, and the mixture evaporated to dryness in vacuo. The residue is taken into 150 ml. 2N NaOH, extracted with CHCl3 to remove undissolved material and adjusted to pH 5 to 6 with 6N HCl to yield 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (V), m. 165-6° (alc.). V in 30 ml. N NaOH treated with Me2SO4 gave I (R1 = iso-Pr, R3 = Me, R4 = PhCH2) (VI), m. 96-7°. The procedure similar to that used for the preparation of IV is used to prepare 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (VII), m. 154-5°. A solution of 1.15 g. Na in 40 ml. absolute alc. is added to 14.4 g. VII in 60 ml. absolute alc. and refluxed 4 hrs. after the addition of 7.5 g. Et2NCH2CH2Cl to give after HCl treatment 15.4 g. III.HCl, m. 147-8°. Similarly, 13.4 g. V is allowed to react with 1.2 g. Na in 300 ml. absolute EtOH, then with 5.5 g. Me2NCH2CH2Cl to yield 10.2 g. I (R1 = iso-Pr, R3 = Me2NCH2CH2, R4 = PhCH2) (VIII), m. 115-17°; VIII.HCl m. 229-31°. V, as the Na salt, is allowed to react with Et2NCH2CH2Cl to yield I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = PhCH2).HCl, m. 202-3°. When V, as the Na salt, is allowed to react with Et2NCH2CH2CHCl, II.HCl, m. 173-5°, is isolated. 1-Methyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (IX) is prepared from 2-methyl-3-amino-4-carbethoxypyrazole and PhCH2CN (X) by the procedure for the preparation of V. The reaction of 12 g. IX with 1.2 g. Na in 25 ml. absolute alc. followed by the addition of 6 g. Et2NCH2CH2Cl leads to the isolation of

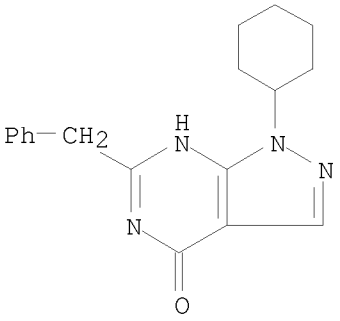
I (R1 = Me, R3 = Et2NCH2CH2, R4 = PhCH2) (XI), m. 83-5° XI.HCl m. 219°. Likewise, 2-phenyl-3-amino-4-carbethoxypyrazole and X yields 1-phenyl-6-benzyl-4-hydroxypyrazolo[3,4-d]pyrimidine, m. 264-5° which is allowed to react as the Na salt with Et2 NCH2CH2Cl to give I (R1 = Ph, R3 =Et2NCH2CH2,CH2, R4 = PhCH2) (XII), m. 103 5° XII.HCl m. 225°. To an ice-cooled solution of 9.9 g. IV in 50 ml. MeCN is added 2.3 g. Na and the temperature of reaction kept below 30°. After the addition, the mixture is heated to 90-95° for 4 hrs., cooled, and 100 ml. EtOH added. The mixture is evaporated to dryness and residue treated with 150 ml. 2N NaOH, extracted with CHCl3 and the aqueous layer adjusted to pH 3 to 4 with 5N HCl and the precipitate crystallized from alc. to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (XIII), m. 195-6°. The reaction of 9.1 g. XII with 1.2 g. Na in 150 ml. absolute alc., followed by the addition of 7 g. Et2NCH2CH2Cl, and 4 hrs. reflux yields 7 g. I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = Me), m. 166-8°. 1,6-Diisopropyl-4-hydroxypyrazolo[3,4-d]pyrimidine (XIV), m. 175-7°, is prepared from iso-BuCN and IV in the presence of Na. A solution of 11 g. XIV in 75 ml. 2N NaOH solution is stirred at room temperature with 6.3 g. Me2SO4 and allowed to stand overnight to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Me), m. 175-7°. XIV (10 g.) is added to a solution of 1.05 g. Na in 150 ml. absolute alc., stirred 1 hr. at room temperature and 6.5 g. Et2. NCH2CH2Cl is added. The mixture is refluxed 4 hrs., evaporated to dryness in vacuo and the residue dissolved in 100 ml. N HCl, adjusted to a pH with NaOH solution and the oil that results is extracted with Et2O. The residue, after removal of the Et2O, is distilled to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Et2NCH2CH2), b0.05 138-40°. A mixture of 20 g. X and 19.7 g. IV is warmed to 70° and 2.3 g. of Na in small pieces added. The mixture is heated 4 hrs. at 110-20°, allowed to cool, and the excess Na destroyed by the addition of alc. The mixture is evaporated to dryness in vacuo, the residue treated with 300 ml. H2O and 2N HCl added to adjust the pH to 3. The precipitate is removed by filtration and crystallized from petr. ether to yield 1-isopropyl-4-hydroxy-6-diphenylmethylpyrazolo[3,4-d]pyrimidine (XV), m. 226 7°. XV(5.2 g.)is added to a solution of 0.35g. Na in 150 ml. EtOH, the mixture stirred at room temperature and 2.1 g. Et2NCH2CH2Cl is added. The mixture is refluxed 4 hrs. and evaporated to dryness in vacuo and the residue crystallized from petr. ether to yield 3.8 g. I (R1 = iso-Pr, R3;= Et2NCH2CH2, R4 = Ph2CH), m. 124-5°.

L5 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:408986 CAPLUS
DOCUMENT NUMBER: 59:8986
ORIGINAL REFERENCE NO.: 59:1635g-h
TITLE: New synthesis of pyrazolo[3,4-d]pyrimidines with dilatory effect on coronary vessels
AUTHOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max; Burckhardt, Christoph A.
CORPORATE SOURCE: CIBA S. A., Basel, Switz.
SOURCE: Annali di Chimica (Rome, Italy) (1963), 53, 61-9
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: French
IT 94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

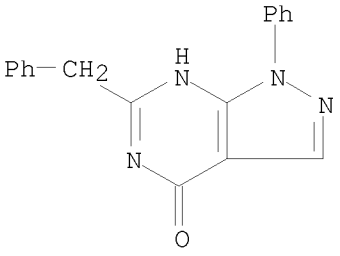


AB cf. Helv. Chim. Acta 45, 1620(1962). The position of the functional groups of 3-amino-4-carbethoxypyrazoles suggested the formation of bicyclic compds. by the action of appropriate reagents. Treatment with suitable nitriles led to a new synthesis of pyrazolo[3,4-d]pyrimidines substituted in the 6-positions, and to 6-aminopyrazolo[3,4-b]pyridines. The reaction was extended to numerous examples and the constitution of the products proved by independent syntheses (exptl. details, loc. cit.). Degradation in acid media converted the 6-substituted pyrazolopyrimidines to pyrazole derivs. Several of the compds. possessed a marked dilatory effect on the coronary vessels.

L5 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:483251 CAPLUS
DOCUMENT NUMBER: 57:83251
ORIGINAL REFERENCE NO.: 57:16611d-i,16612a-e
TITLE: Chemotherapeutic studies in the heterocyclic series. XXXIV. Pyrazolopyrimidines. 5. A new synthesis of pyrazolo[3,4-d]pyrimidine with coronary dilating properties
AUTHOR(S): Schmidt, P.; Eichenberger, K.; Wilhelm, M.
CORPORATE SOURCE: Ciba, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1962), 45, 1620-7
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 57:83251
IT 94068-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 94068-86-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclohexyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)

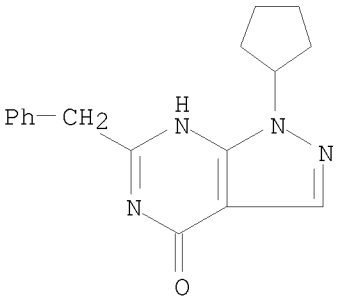


IT 94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-phenyl- 97433-46-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1-cyclopentyl-1,5-dihydro-
RL: PREP (Preparation)
(preparation of)
RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



RN 97433-46-0 CAPLUS

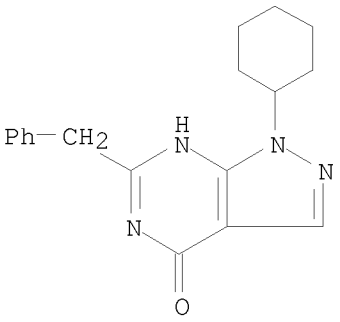
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



AB cf. CA 53, 20070d. The condensation of 3-amino-4-carbethoxypyrazoles with nitriles led to a new synthesis of 6-(C-substituted) pyrazolo[3,4-d]pyrimidines (I) and 6-aminopyrazolo[3,4-b]pyridines. The I could be cleaved with H3PO4 to 3-aminopyrazole-4-carboxamide derivs. Many of the new I caused an increase of coronary flow. 2-Isopropyl-3-amino-4-carbethoxypyrazole (II) (19.7 g.) in 250 cc. 2N NaOH refluxed 2 hrs., cooled, treated with C, and acidified with concentrated HCl to pH 3-4 gave 14.5 g. 4-CO2H analog (III) of II, m. 151-2° (decomposition). III (84.5 g.) in 375 cc. dioxane and 40 cc. C5H5N treated dropwise with stirring at 10-15° with 77.3 g. PhCH2COCl in 125 cc. dry dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, diluted with H2O and aqueous HCl, and extracted with Et2O gave 53 g. 2-isopropyl-3-phenylacetylamino-4-carboxypyrazole (IV), m. 162-3°. IV (8.61 g.) and 30 cc. Ac2O stirred 3 hrs. at 100-10° and evaporated yielded 3.1 g. 1-isopropyl-4-oxo-6-benzylpyrazolo[3,4-d]oxazine (V), m. 162-3° (Me2CO-petr. ether). III (30 g.) in 180 cc. dry dioxane and 16 cc. C5H5N treated dropwise with stirring at 10-15° with 31 g. PhCH2COCl in 50 cc. dioxane and processed in the usual manner gave 21 g. 4-CN analog (VI) of IV, m. 140-2° (EtOH). PhCH2CN (26.3 g.) in 250 cc. CHCl3 and 13 cc. absolute EtOH saturated with dry HCl, kept overnight, evaporated below 30°, the residue dissolved in 200 cc. CHCl3, treated with 16.9 g. 2-isopropyl-3-amino-4-carbamoylpyrazole (VII) in 1800 cc. CHCl3, refluxed 10 hrs. with stirring, filtered, and evaporated yielded 2-isopropyl-3-(1-ethoxy-2-phenylethylidenimino)-pyrazole-4-carboxamide (VIII), m. 111-14° (Et2O). II (70 g.) and 140 g. PhCH2CN added during 1 hr. with stirring at 90-5° to 16.5 g. powdered Na in 300 cc. dry MePh, refluxed 7 hrs. with stirring, diluted with 240 cc. absolute EtOH, evaporated, the residue dissolved in 1.2 l. N NaOH, washed with MePh, and acidified with 5N HCl to pH 5-6 gave 62.4 g. 1-isopropyl-4-oxo-6-benzyl-4,5-dihydropyrazolo [3,4 - d]pyrimidine (IX), m. 164-6° (absolute EtOH); the alc. mother liquor concentrated, filtered, the residue (8.1 g.) shaken 0.5 hr. with 81 cc. CH2Cl2, and filtered left 4.77 g. 2-isopropyl-4-hydroxy-5-phenyl-6-aminopyrazolo[3,4-b]pyridine (X), m. 256-7° (EtOH); the CH2Cl2 filtrate evaporated gave 1.9 g. IX. Similarly were prepared the following 1,6-disubstituted-4-oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (1- and 6-substituent and m.p. given): Me, PhCH2, 233-7°; Me, p-ClC6H4CH2, 268-70°; Me, 3,4,5-(MeO)3C6H2CH2, 245-6°; HOCH2CH2, PhCH2, 194-5°; iso-Pr, Me, 180-2°; iso-Pr, Ph, 256-8°; iso-Pr, PhCH2, 165-6°; iso-Pr, p-EtOC6H4CH2,

175-6°; cyclopentyl, PhCH2, 189-90°; cyclohexyl, PhCH2, 207-8°; Ph, PhCH2 (XIII), 263-5°. V (5.4 g.), 50 cc. C6H6, and 15 cc. liquid NH3 in a sealed tube heated 8 hrs. at 100-10°, treated with 2N NaOH, and the aqueous phase acidified with 6N HCl to pH 6 gave 0.7 g. IX. VI(6.7g.) and 27.2 cc. 10% aqueous KOH in 102 cc. 3% H2O2 heated 10 hrs. at 70°, filtered, and acidified with 2N HCl to pH 5 yielded 6.12 g. IX, m. 163-5°. Crude VIII from 26.3 g. PhCH2CN and 16.9 g. VII added to 18 g. Na in 315 cc. MeOH, kept overnight, refluxed 0.5 hr., filtered, evaporated, the residue shaken with 200 cc. H2O and 200 cc. CHCl3, and the aqueous phase acidified with 5N HCl gave 16.6 g. IX. VII (8.4 g.) and 27 g. PhCH2CONH2 heated 4 hrs. at 200-10°, cooled, powdered, extracted with 2N NaOH, and the alkaline extract acidified with 2N HCl to pH 3 yielded 3.2 g. IX, m. 165-6° (EtOH). II (39.4 g.) in 150 cc. dry dioxane and 16 cc. C5H5N treated with stirring at 10-15° during 15 min. with 31 g. PhCH2COCl in 50 cc. dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, treated with 130 cc. 2N HCl and 380 cc. H2O, and extracted with about 1000 cc. Et2O yielded 33 g. 2-isopropyl-3-phenylacetylamino-4-carbethoxypyrazole (XIV), b0.08 170-5°. NaNO2 (7 g.) and 26.8 g. X added successively with stirring at 0-5° to 268 cc. concentrated H2SO4, stirred 3 hrs. at 0-5°, cooled, poured onto ice, heated with stirring to 80°, cooled, filtered, the residue (about 20 g.) treated with 400 cc. saturated aqueous NaHCO3 and 400 cc. H2O, filtered, and the filtrate acidified with 2N HCl to pH 3-4 yielded 16.8 g. 1-isopropyl-4-hydroxy-5-phenyl- 6-oxo-4,5-dihydropyrazolo[3,4-b]pyridine (XV), m. 322-4° (EtOH). XIV (10 g.) and 2 g. Na in 150 cc. MePh refluxed 5 hrs. with stirring, cooled to room temperature, treated with EtOH, evaporated, the residue dissolved in H2O, washed with Et2O, and acidified with 2N HCl gave 2.3 g. XV, m. 322-4° (aqueous EtOH). XIII (15 g.) and 100 cc. POCl3 refluxed 6 hrs., evaporated, the residue dissolved in CHCl3, and worked up gave 7.2 g. 1-phenyl-4-chloro-6-benzylpyrazolo[3,4-d]pyrimidine (XVI), m. 90-1° (CHCl3-petr. ether). XVI (7 g.) and 25 g. Me2NH in 50 cc. EtOH heated 7 hrs. at 100° in an autoclave gave 4.3 g. 4-Me2N analog of XVI, m. 121-2° (EtOH). IX (13.4 g.) and 1.15 g. Na in 300 cc. EtOH stirred 1 hr. at room temperature, treated with 5.5 g. Me2NCH2CH2Cl, refluxed 4 hrs., evaporated, the residue dissolved in 100 cc. N HCl, washed with Et2O, basified to pH 10 with aqueous NaOH, and extracted with Et2O yielded 13 g. 5-Me2NCH2CH2 derivative (XVII) of IX, m. 115-17° (petr. ether). XVII (10 g.) and 35 cc. 85% H3PO4 stirred 6 hrs. at 100°, poured onto 300 g. ice, adjusted with aqueous NaOH to pH 10, filtered, and extracted with CHCl3 gave 6 g. 2-isopropyl-3-aminopyrazole-4-carboxylic acid 2-dimethylaminoethylamide, m. 131-2° (iso-Pr2O).

L5 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:483250 CAPLUS
DOCUMENT NUMBER: 57:83250
ORIGINAL REFERENCE NO.: 57:16609h-i,16610a-i,16611a-d
TITLE: Chemotherapeutic studies in the heterocyclic series. XXXIII. 1-Aryl-2-alkyl-3,6-dioxo-1,2,3,6-tetrahydropyridazines
AUTHOR(S): Druey, J.; Meier, Kd.; Staehelin, A.
CORPORATE SOURCE: Ciba, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1962), 45, 1485-98
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 57:83250
IT 94068-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 94068-86-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclohexyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



AB cf. CA 57, 11157a. Several 1,2-disubstituted 3,6-dioxo-1,2,3,6-tetrahydropyridazines (I) were prepared Direct alkylation of 1-aryl-3-hydroxy-6-oxo-1,6-dihydropyridazines (II) with dialkyl sulfates gave either 1-aryl-2-alkyl-3,6-dioxo-1,2,3,6-tetrahydropyridazines (III) or a mixture of the III with the 3-alkyl ethers (IV) of II. Ph-NHNH2 (162 g.), 2.5 l. H2O, 365 g. 30% HCl, and 147 g. maleic anhydride (V) refluxed 4 h. with stirring, cooled to room temperature, and filtered yielded 225 g. yellowish crystalline 1-phenyl-3-hydroxy-6-oxo-1,6-dihydropyridazine, m. 262-3°. Similarly were prepared the following II (aryl group and m.p. given): p-MeC6H4 (VI) 242-4°, p-MeOC6H4 - (used crude), o-ClC6H4 (VII) 269-70°, m-ClC6H4 249-51°, p-ClC6H4 (VIII) 280-2°. II (100 g.) and 80 cc. Me2SO4 stirred 2.5 h. at 150°, stirred into 67.5 g. Na2CO3 in 1200 cc. H2O, stirred several hrs., and extracted with CHCl3 gave 96.1 g. 1-phenyl-2-methyl-3,6-dioxo-1,2,3,6 -tetrahydropyridazine (VIIIa), m. 173-5° (EtOAc-MeOH). Similarly were prepared the following I (2-substituent = Me) (1-substituent reaction time, reaction temperature and, m.p. given): p-MeC6H4, 132-4°, 5 h., 145-50°; p-MeOC6H4, 138.5-40°, 5-10 min., 190-200°; o-ClC6H4, 107-8°, 10 min., 190-200°; m-ClC6H4, 139-41°, 4 h., 150-5°; p-ClC6H4, 145-6°, 35 min., 150-200°. In the same manner were obtained the following 4(or 5)-substituted III (aryl = Ph, alkyl = Me) (substituent, m.p., reaction time, and reaction temperature given): 4-MeO, 118.5-19.5°, 0.5

h., 140-50° [and the 3-Me ether of the 4-MeO derivative of II (aryl = Ph), m. 157-8°], 4-Me, 111-13°, 1.5 h., 140-50° [and the 3-Me ether of the 4-Me derivative of II (aryl = Ph), m. 117-18°]; 4-Cl, 150-2°, 3.5 h., 140-50°; 5-MeO, 156.5-7.5°, 4 h., 140-5°; 5-Me, 129-31°, 10 min., 190-200°; 5-Cl, 156-7.5°, 3.5 h., 140-50°. 1-Phenyl-3-hydroxy-4-chloro-6-oxo-1,6-dihydropyridazine (IX) (23 g.) in 300 cc. boiling MeOH treated dropwise during 45 min. with 9.2 g. Na in 200 cc. MeOH, refluxed 8 h., diluted with H2O, concentrated, filtered through C, acidified with AcOH, and cooled gave 18.4 g. 4-Me ether of IX, m. 260-2° (decomposition) (EtOH). 1-Phenyl-3-hydroxy-5-chloro-6-oxo-1,6-dihydropyridazine (X) (3.5 g.), 1 g. Na, and 100 cc. absolute MeOH heated 12 h. at 120-30° in a sealed tube, evaporated, the residue treated with 2N HCl, and filtered gave 2.2 g. 5-Me ether of X, m. 244-7° (MeOH). II (300 g.) and 300 cc. Et2SO4 heated 15 min. at 190-200°, cooled, stirred into 2 l. saturated aqueous Na2CO3, diluted with 2 l. H2O, stirred 4 h., and extracted with Et2O gave 120 g. (crude) 3-Et ether (XI) of II, m. 86-7° (EtOH); the aqueous phase extracted with CHCl3 gave 126 g. 1-phenyl-2-ethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine (XII), m. 121-3° (cyclohexane); the alkaline aqueous mother liquor acidified gave 50 g. unchanged II. Similarly were prepared the following IV and III (R = Et) (aryl group and m.p. of IV and III given): o-ClC6H4, 114-16°, 100-2°; p-ClC6H4, 141-2°, 142.5-43°; p-MeC6H4, 108-10°, 119-21°. MeNHNHPh.HCl (XIII.HCl) (9 g.) and 5.6 g. V in 60 cc. H2O heated with stirring on the water bath to solution, kept 3 days at room temperature, and extracted with CHCl3 yielded 1.7 g. VIIIa; the aqueous phase basified and extracted with Et2O yielded 4.6 g. unreacted XIII. Maleic acid mono-N-methyl-N'-phenylhydrazide (XIV) (10 g.) in 80 cc. Ac2O refluxed 0.5 h. gave 7.3 g. pale yellow crystalline II, m. 178-9.5° (MeOH). XIV (10 g.) in 100 cc. 33% HCl-MeOH kept 5 days at room temperature, evaporated, the residue treated with H2O, and extracted with CHCl3 gave 8.6 g. II, m. 173-6°. VIIIa (100 g.) in 1.4 l. absolute EtOH hydrogenated 20 min. at 40° over 10 g. Raney Ni gave 96.2 g. 1-phenyl-2-methyl-3,6-dioxohexahydropyridazine (XV), m. 143-5° (4:1 MeOH-H2O). HO2CCH2CH2CONMeNHPh (5 g.) in 10 cc. Ac2O refluxed 2 h., cooled, poured into H2O, kept 4 h., and filtered yielded 2.7 g. XV, m. 144-7.5°; 2.0 g. 2nd crop. VIIIa (2050 g.) in 3000 cc. AcOH treated during 1 h. at 80-5° with stirring with 1620 g. Br in 100 cc. AcOH, kept several hrs. at 5°, and filtered yielded 3176 g. 1-phenyl-2-methyl-3,6-dioxo-4,5-dibromohexahydropyridazine (XVI), m. 177-8.5° (decomposition) (MeOH). XVI (108 g.) and 35.5 g. C5H5N in 370 cc. CHCl3 refluxed 6 h. gave 81 g. (crude) 1-phenyl-2-methyl-5-bromo-3,6-dioxo-1,2,3,6 -tetrahydropyridazine (XVII), m. 159-61° (MeOH). VIIIa (15 g.) in 200 cc. AcOH stirred 2.5 h. on the water bath while being treated with Cl, the mixture evaporated, the residue diluted with H2O, and extracted with CHCl3 yielded 4.1 g. 4,5-di-Cl analog (XVIII) of XVI, m. 134-6° (MeOH). XVIII (0.9 g.) and 0.5 g. C5H5N in 15 cc. CHCl3 refluxed 6 h. yielded 0.75 g. 5-Cl analog (XIX) of XVII, m. 154-6° (MeOH). VIIIa (10.1 g.) in 250 cc. dry dioxane and 100 cc. MePh kept 4 wk at room temperature with 13 g. cyclopentadiene and a trace methylene blue, evaporated, and the residue (14.8 g.) recrystd. from MeOH gave 5.9 g. 2-phenyl-3-methyl-5,8-endomethylene-1,4-dioxo-1,2,3,4,4a,5,8,8a-octahydrophthalazine, m. 127-7.5°. VIIIa (202 g.) in 1 l. 2N HCl

refluxed 12 h., cooled, filtered from 60.3 g. fumaric acid, m. 285-7°, and extracted with $CHCl_3$ gave 27.2 g. unreacted VIIIa; the aqueous phase basified with cooling with 10N NaOH and extracted with Et_2O yielded 86.5 g. (crude) XIII, leaflets, m. 164-7° (absolute EtOH-Et_2O). VIIIa (101 g.) added with stirring at 30-5° to 20 g. NaOH in 500 cc. H_2O, stirred 4 h., filtered, the filtrate extracted with $CHCl_3$, and the extract evaporated gave 3.3 g. unreacted VIIIa; the filter residue dissolved at 30-40° with stirring in the $CHCl_3$-extracted filtrate and acidified with 6N HCl gave 84.6 g. XIV, m. 105-7° (EtOAc-petr. ether). XIII (6.1 g.) and 4.9 g. V in 50 cc. $CHCl_3$ kept several hrs. at room temperature, extracted with 2N aqueous Na_2CO_3, the extract acidified with 6N HCl, and extracted with $CHCl_3$ gave 7.0 g. VIIIa, m. 106-9°. XV (10.2 g.), 2.0 g. NaOH, and 150 cc. H_2O stirred 4 h. at room temperature and extracted with Et_2O gave 0.2 g. unchanged XV; the aqueous phase acidified and extracted with $CHCl_3$ yielded 10.5 g. (crude) XIV, m. 126-8°. XIV (44 g.) in 1 l. absolute EtOH hydrogenated under ambient conditions over 5 g. Raney Ni gave 40.5 g. XV, m. 124-6°. XV (10 g.) in 80 cc. morpholine refluxed 6 h. gave 15.5 g. morpholide of XV, m. 99-101° (Me_2CO-petr. ether). XV (20 g.) and 150 cc. liquid Me_2NH heated 6 h. in a sealed tube at 100-10° gave 25.3 g. (crude) dimethylamide of XV, m. 98-100° (Me_2CO-petr. ether). XV (5 g.) and 20 cc. $N_2H_4.HCO$ refluxed 6 h., evaporated, the residue diluted with H_2O, and extracted with $CHCl_3$ gave 1.5 g. XIII, m. 160-2°; the aqueous phase evaporated gave 2.2 g. $(CH_2CONHNH_2)_2$, m. 164-6° (aqueous EtOH). XVII (562 g.) and 84 g. NaOH in 4 l. H_2O stirred 4 h. at room temperature, filtered, and extracted with $CHCl_3$ gave 64 g. unreacted XVII, m. 224-6° (decomposition); the filtrate concentrated gave 515 g. Na salt (XX) of β-bromomaleic acid mono-N-methyl-N'-phenylhydrazide (XXI); the aqueous mother liquor acidified with HCl gave 26 g. 1-phenyl-2-methyl-3-pyrazolone-5-carboxylic acid (XXII), m. 198-200° (absolute EtOH). XX in H_2O acidified with HCl gave XXI, m. 135-7° (decomposition) (EtOAc). XX (215 g.) and 120 g. morpholine in 860 cc. H_2O refluxed 1.5 h., filtered hot, and acidified with HCl gave 131 g. XXII, m. 200.5-2.5° (decomposition) (absolute EtOH).

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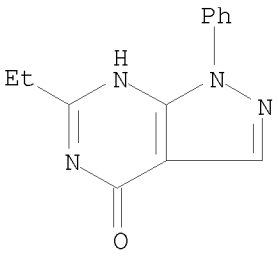
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.
AB cf. C.A. 52, 13741h. A synthesis of 6-alkyl-4-hydroxypyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:COH (I) was devised from the corresponding 5-acylamino-4-cyanopyrazoles, R3CONHC:C(CN).CR2:N.NR1 (II) which were in turn prepared from 5-amino-4-cyanopyrazoles, R1N.N:CH.C(CN):CNH2 (III). Evidence was presented to show that the 5-acylaminopyrazole-4-carboxamide is an intermediate in this cyclization. Chlorination of I yielded the corresponding 6-alkyl-4-chloropyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CCl (IV). Nucleophilic displacement of the Cl in IV resulted in the preparation of a large number of 6-alkylpyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CNR4R5 (V). III (R1 = 3-Me) (80 g.) and 250 ml. Ac2O refluxed 10 hrs., excess Ac2O distilled in vacuo, the sirupy substance poured into 30 ml. C6H6, stirred several min., and crystallized gave 89 g. II (R1 = R2 = H, R3 = Me), crystals from H2O. Similarly II (R1 = R3 = Me, R2 = H) was prepared and the product recrystd. from H2O to a white powder. III (R1 = Ph) (150 g.) treated 19 hrs. under reflux with 200 ml. Ac2O, excess solvent removed, the residue treated with a small amount of C6H6, and Skellysolve (b. 60°), and the product isolated gave 171 g. II (R1 = Ph, R2 = H, R3 = Me) crystallized from H2O. The following II were thus prepared (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, H, Me, 221-2°, 76, H2O; Me, H, Me, 210-11°, 72, H2O; Ph, H, Me, 155-6°, 92, H2O; o-ClC6H4, H, Me, 175-5.5°, 82, alc., H2O; p-ClC6H4, H, Me, 173-5°, 96, alc, H2O; p-BrC6H4, H, Me, 175-5° (sic), 98, alc., H2O; p-O2NC6H4, H, Me, 198-200°, 95, alc., H2O; p-MeC6H4, H, Me, 128°, 96, alc., H2O; AcOCH2CH2, H, Me, 155-7°, 81, alc.

II (R1 = Ph, R2 = H, R3 = Me) (30 g.) added at 15-20° to 120 ml. concentrated H2SO4, the clear solution stirred 0.5 hr., then poured onto 1 kg. ice, neutralized with concentrated NH4OH, the solid collected, washed, dried, and recrystd. from C6H6 and MeOH gave 20 g. 5-amino-1-phenylpyrazole-4-carboxamide (VI), m. 172-5°, identical with the product obtained from the hydrolysis of 5-amino-4-cyano-1-phenylpyrazole. VI (20 g.) and 200 ml. Ac2O refluxed 15 hrs., and purification gave 15 g. 6-methyl-4-oxo-1-phenylpyrazolo [3,4-d]-5,7-oxazine (VII), m. 184.5-5.5° (sublimed at 145°) (C6H6-C7H16). VII (2.5 g.) kept 2 hrs. at room temperature with 200 ml. H2O and 2 g. KOH, heated 10 hrs., acidified, and the precipitate collected gave 2 g. 5-acetamido-1-phenylpyrazole-4-carboxylic acid (VIII), m. 201-2° (AcOH), readily lost CO2 on heating. The 5-acetylamido group was retained in warm alkaline solution but hydrolyzed readily in cold acidic medium. VII (2 g.) left 0.5 hr. at room temperature with 100 ml. alc. NH3, heated briefly until a solid product precipitated, and the product collected gave 5-acetamido-1-phenylpyrazole-4-carboxamide (IX), m. 301-2°, relatively unstable. The m.p. of IX was the same as that for I (R1 = Ph, R2 = Me) and was undepressed in mixed m.p. The ultraviolet absorptions for IX at 230 mμ and for I at 233 and 269 mμ, were different. Thus IX cyclized at elevated temps. during the m.p. determination I were prepared by the following method. II (R1 = R2 = H, R3 = Me) (1.5 g.); 7 ml. 10% KOH, and 15 ml. 3% H2O2 warmed 0.5 hr. at 70-5°, the mixture acidified, the solid collected, and repptd. with dilute KOH and AcOH gave 1.1 g. I (R1 = H, R2 = Me). II (R1 = R3 = Me, R2 = H) (121 g.) warmed 10 hrs. at 70° with 1500 ml. 3% H2O2 and 400 ml. 10% KOH gave 103 g. I (R1 = R2 = Me), needles, sublimed at 180°. II (R1 = Ph, R2 = H, R3 = Me) (14.5 g.) in 5 g. KOH and 200 ml. 3% H2O2 warmed 5 hrs. at 70-5° and acidified gave 14 g. crude I (R1 = Ph, R2 = Me), m. 298-300°. IX(1 g.) heated 20 min. at 70° with 100 ml. 10% KOH, then acidified, the solid collected and recrystd. gave 0.8 g. product identical with that from the preceding experiment I (R1 = R2 = Me) (25 g.) and 400 ml. POCl3 refluxed 2 hrs., excess solvent removed, the sirup poured onto 1 kg. ice, the suspension left 15 min., extracted with CHCl3, dried, solvent removed at room temperature, and the solid isolated gave 24 g. IV (R1 = R2 = Me) as needles. I (R1 = H, R2 = Me)(50 g.) refluxed 2 hrs. with 140 ml. PhNMe2 and 1 l. POCl3, excess POCl3 removed, the residue poured on ice, and extracted with Et2O gave 35 g. IV (R1 = H, R2 = Me), unstable. I (R1 = p-O2NC6H4, R2 = Me) (20 g.) refluxed 3 hrs. with 250 ml. POCl3 gave 17.5 g. IV (R1 = p-O2NC6H4, R2 = Me) as a yellow powder. Preparation of 1-alkyl(aryl)-6-alkyl-4-mercaptopyrazolo[3,4-d]pyrimidines X) (R1 = 1-substituent, R2 = 6-substituent) was achieved by the following two methods: (method 1) I (R1 = Ph, R2 = Me) (11 g.) and 50 g. P2S6 added portionwise during 45 min. to 400 ml. Tetralin (preheated to 165°), the temperature allowed to rise to 185°, then heated 6 hrs. to 190-5°, the solution cooled overnight, filtered, the product dissolved in dilute KOH and precipitated with AcOH gave 5.5 g. X (R1 = Ph, R2 = Me); method 2) IV (R1 = Ph, R2 = Me) (14 g.) and 14 g. CS(CH2)2 in 120 ml. alc. refluxed 4 hrs., the product collected and washed well with alc. and H2O, and the product purified by precipitation from a hot basic solution with AcOH gave 11.5 g. X (R1 = Ph, R2 = Me). All the other X were prepared by essentially the same procedure as method 2. 1-Alkyl(aryl)-6-alkyl-4-

alkylthiopyrazolo[3,4-d]pyrimidines (XI) (R1 = 1-substituent, R2 = 6-substituent, R3 = S-substituent were prepared as follows: X (R1 = R2 = Me) (13 g.), 40 ml. 4N KOH, 18 g. MeI, and 30 ml. MeOH shaken 0.5 hr. in a separatory funnel, the contents left overnight at 40°, and the solid collected gave 12.5 g. XI (R1 = R2 = R3 = Me). X (R1 = Ph, R2 = Me) (1 g.) added to 200 ml. H2O containing 15 g. KOH and 21 g. EtI, treated with 100 ml. alc., refluxed 5 hrs., and reduced in volume, until an oily product solidified gave 3 g. XI (R1 = Ph, R2 = Me, R3 = Et). 4-Alkoxy-1-alkyl(aryl)-6-methylpyrazolo[3,4-d]pyrimidines (XII) (R1 = 1-substituent, R2 = O-substituent) were prepared as follows: IV (R1 = p-MeC6H4, R2 = Me) (5.5 g.) and 100 ml. alc. left 2 hrs. at room temperature with 2 g. Na in 70 ml. alc., heated 40 min. on the steam bath, and NaCl removed, the filtrate treated with 50 ml. H2O, and left overnight in the cold gave 3.1 g. XII (R1 = p-MeC6H4, R2 = Et). Other XII were prepared as above. The following N:CR2.N:CR3.C:C.NR1.N:CH were prepared by the above methods (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, Me, 0H, 336-8°, 73.5, AcOH; H, Me, Cl, 140° (decomposition), 70.0, C6H6; H, Me, SH, above 300°, 80, repptd.; H, Et, OH, above 300°, 82, alc., H2O; Me, Me, OH, 277-8°, 72.5, alc., H2O; Me, Me, Cl, 74°, 70.2, C7H16; Me, Me, OMe, 107.5-8.5°, 67.5, MeOH; Me, Me, SH, 264-5°, 98, repptd.; Me, Me, SMe, 74-5°, 90.2, MeOH, H2O; CH2CH2OH, Me, OH, 265-6°, 54.8, H2O; Ph, Me, Cl, 85-6°, 83.5, C7H16; Ph, Me, SH, 268.5°, 83.3, repptd.; Ph, Me, OMe, 121.5-2.0°, -, MeOH; Ph, Me, OEt, 95-5.5°, -, alc.; Ph, Me, SMe, 135-7°, -, MeOH, H2O; Ph, Me, SEt, 86-8°, -, alc., H2O; Ph, Et, OH, 295°, 88.5, alc., H2O; Ph, Et, SH, 248-9°, 91.6, repptd.; p-MeC6H4, Me, OH, 298-300°, 93.6, alc., H2O; p-MeC6H4, Me, Cl, 89-91°, 78.1, C7H16; p-MeC6H4, Me, OMe, 121-2°, 81.2, MeOH; p-MeC6H4, Me, OEt, 93-4°, 53, alc.; o-ClC6H4, Me, Cl, 121°, 77.8, C6H14; p-BrC6H4, Me, OH, above 315°, 86.6, alc., H2O; p-BrC6H4, Me, Cl, 130.5-31°, 88.7, C6H14; p-ClC6H4, Me, OH, above 310°, 94.5, alc., H2O; p-ClC6H4, Me, Cl, 129°, 82.6, C7H16; p-ClC6H4, Me, SH, above 305°, 75.2, repptd.; p-O2NC6H4, Me, OH, above 310°, 90, repptd.; p-O2NC6H4, Me, Cl, 184°, 82, PhMe. V were prepared by the following methods: (method A) IV (R1 = H, R2 = Me) (10 g.) and 120 ml. alc. NH3 heated 8 hrs. in a bomb at 160°, the product evaporated to dryness, the residue refluxed with dilute HCl, the solution treated with C, filtered, and the product repptd. with NH4OH, filtered, and recrystd. gave 6.5 g. V (R1 = R4 = R5 = H, R2 = Me); (method B) the above IV (5 g.) added to 7 g. BuNH2, and 120 ml. alc. and the mixture refluxed 7 hrs. gave 3 g. V (R1 = R4 = H, R2 = Me, R5 = Bu). IV (R1 = Ph, R2 = Me) (5 g.) refluxed 40 min. with 8 g. p-ClC6H4NH2 and 75 ml. alc. and the mixture filtered after cooling 3 hrs. in an ice bath gave 6.2 g. crude V (R1 = Ph, R2 = Me, R4 = H, R5 = p-ClC6H4). IV (R1 = p-ClC6H4, R2 = Me) (9 g.) refluxed on a steam bath to near dryness with 160 ml. alc. containing 10 g. PhCH2CH2NH2 and the residue added to MeOH gave 11 g. V (R1 = p-ClC6H4, R2 = Me, R4 = H, R5 = CH2CH2Ph); (method C) IV (R1 = R2 = Me) (5.5. g.), 5.5 g. furfurylamine, and 200 ml. alc. heated 8 hrs. on a steam bath, then evaporated, the residue stirred with 30 ml. 10% KOH, the alkaline solution decanted, the sirup refluxed 2 hrs. with 100 ml. C6H6, and the solution, filtered and evaporated to dryness gave 4 g. V (R1 = R2 = Me, R4 = H, R5 = furfuryl as white needles. IV (R1 = Ph, R2 = Et) (13 g.) in 150 ml. alc. treated slowly with 13 g. PhCH2NH2 in 50 ml. alc., the mixture refluxed 12 hrs., the solvent removed, and the product treated with C6H6 and several drops MeOH, and refrigerated gave 8 g. V (R1 = Ph, R2 = Et, R4 =

H, R5 = CH2Ph). The following V were prepared by these methods (R1, R2, R4, R5, m.p., method of preparation, % yield, and recrystn. solvents given): H, Me, H, H, above 300°, A, 73, alc., H2O; H, Me, H, Me, above 300°, B ,60, alc., H2O; H, Me, H, Et, 273-4°, B, 56, alc.; H, Me, H, Pr, 220-2°, B, 49.1, alc.; H, Me, H, CH2Ph, 241°, B, 87.2, alc.; H, Me, H, furfuryl, 243-4°, C, 59, alc.; Me, Me, H, H, 251-2°, A, 90, alc., H2O; Me, Me, H, Me, 136-8°, B, 77.2, H2O; Me, Me, H, Et, 131.5-2.0°, C, 66.9, PhMe, C7H16; Me, Me, H, CH2Ph, 180-2°, B, 83, alc.; Me, Me, H, furfuryl, 140-1.5°, C, 54.6, alc.; Me, Me, H, o-ClC6H4, 223.5-4.0°, B, 60, alc.; Me, Me, H, p-ClC6H4, 231.5°, B, 67, alc., H2O; Me, Me, H, p-MeC6H4, 224-5.5°, B, 60, alc.; Me, Me, H, p-MeC6H4, 225-7°, B, 74.7, alc.; Me, Me, H, 2,6-Et2C6H3, 218-18.5°, B, 48.5, alc.; Me, Me, H, NH2, 259-60°, B, 87.3, alc.; Ph, Me, H, H, 287-9°, A 82.5, alc., H2O; Ph, Me, H, Me, 162-3°, B, 80.2, alc., H2O Ph, Me, Me, Me, 117-17.5°, C, 82.5, alc.; Ph, Me, H, Et, 86°, B, 87.2, alc.; Ph, Me, Et, Et, 66-8°, C, 83, alc.; Ph, Me, H, iso-Pr 143-4°, B 86, alc., H2O; Ph, Me, H, tert-Bu, 175-7°, C, 61, alc., H2O; Ph, Me, H, CH2CH2NEt2, 159-60°, C, 49.1, C7H16; Ph, Me, CH2Ph, H, 187-8°, B, 92, alc.; Ph, Me, H, furfuryl, 153-4.5°, C, 56.2, PhMe, C7H16; Ph, Me, H, Ph, 262-3°, B, 50.5, EtOCH2CH2OH; Ph, Me, H, m-BrC6H4, 215-17°, B, 68, alc.; Ph, Me, H, o-ClC6H4, 175-6°, B, 51.3, alc.; Ph, Me, H, m-ClC6H4, 192-3°, B, 90, alc.; Ph, Me, H, p-ClC6H4, 226-6.5°, B, 82, alc., H2O; Ph, Me, H, 2,6-Et2C6H3, 189-90°, B, 71.2, alc.; Ph, Me, H, NH2, 243-4°, B, 80.1, C5H5N; Ph, Me, H, NHPh, 240-1°, B, 47.5, C5H5N; Ph, Et, Me, Me, 90.5-1.0°, B, 55.5, alc.; Ph, Et, H, tert-Bu, 148-8.5°, C 73.3, alc. (sublimed); Ph, Et, H, CH2Ph, 129-9.5°, C, 48.5, C, 48.5, C6H6, alc.; Ph, Et, H, o-ClC6H4, 168-8.5°, B, 71.5, EtOCH2CH2OH; Ph, Et, H, m-ClC6H4, 187-9°, B, 74, alc.; Ph, Et, H, p-ClC6H4, 208.5-9.5°, B, 87.8, EtOCH2CH2OH; Ph, Et, H, o-MeC6H4, 175-6°, B, 75.5, alc.; Ph, Et, H, m-MeC6H4, 169.5°, B, 58, alc.; Ph, Et, H, p-MeC6H4, 199-200°, B, 78.6, alc.; Ph, Et, H, 2,5-Cl2C6H3, 181-3°, B, 42.1, alc.; Ph, Et, H, 2,6-Et2C6H3, 191-1.5°, B, 38, alc.; Ph, Et, H, NH2, 198-9°, B, 87.5, alc.; p-MeC6H4, Me, H, H, 296.5-8.0°, A, 75.7, alc.; p-MeC6H4, Me, H, Me, 181-2.5°, B, 86, MeOH, H2O; p-MeC6H4, Me, Me, Me, 149-51°, B, 82.2, alc.; p-MeC6H4, Me, H, Et, 144-6°, B, 80, alc., H2O; p-MeC6H4, Me, H, CH2CH2NEt2, 165°, C, 62.8, PhMe, C7H16; p-MeC6H4, Me, H, o-ClC6H4, 219-21°, B, 76.5, C5H5N; p-MeC6H4, Me, H, m-BrC6H4, 218-20°, B, 63.5, alc.; o-ClC6H4, Me, H, H, 294.5-9.5°, A, 71.8, alc.; o-ClC6H4, Me, Me, Me, 152-3°, C, 77.7, alc.; o-ClC6H4, Me H, o-ClC6H4, 196-8°, B, 63, alc.; p-BrC6H4, Me, Et, Et, 123-4°, B, 51.6, EtOCH2CH2OH, H2O; p-ClC6H4, Me, H, H, above 300°, A, 36, alc.; p-ClC6H4, Me, H, Me, 218-19°, B, 57.2, alc.; H2O; p-ClC6H4, Me, H, iso-PrO(CH2)3, 109-10°, B, 51.1, MeOH, H2O; p-ClC6H4, Me, (R4R5 =) (CH2)5, 127.5-8.5°, B, 61.3, alc., H2O; p-ClC6H4, Me, H, CH2Ph, 214°, B, 93.3, EtOCH2CH2OH; p-ClC6H4, Me, H, CH2CH2Ph, 175-6°, B, 60.1, alc.; p-ClC6H4, Me, H, o-ClC6H4, 221-2°, B, 62.0, C5H5N, p-ClC6H4, Me, H, m-ClC6H4, 222-3°, B, 85.5, EtOCH2CH2OH; p-ClC6H4, Me, H, p-ClC6H4, 239-9.5°, B, 88, C5H5N; p-ClC6H4, Me, H, m-BrC6H4, 230-2°, B, 74.2, C5H5N; p-ClC6H4, Me, H, 2,5-Cl2C6H3, 200°, B, 71.5, EtOCH2CH2OH; p-O2NC6H4, Me, H, Me, 248-9°, B, 69, alc.; p-O2NC6H4, Me, Me, Me,

196°, B, 51.2, alc., H2O; p-O2NC6H4, Me, H, iso-Pr, 190-2°, B, 81.1, alc.; p-O2NC6H4, Me, H, Bu, 147°, B, 66.6, alc.; p-O2NC6H4, Me, (R4R5 =) (CH2)5, 189-91°, B, 96, C5H5N; p-O2NC6H4, Me, H, CH2CH2NEt2, 145°, B, 91.7, alc., H2O; p-O2NC6H4, Me, H, o-ClC6H4, 227-8°, B, 43.2, alc.; p-O2NC6H4, Me, H, p-ClC6H4, 278°, B, 87, AcOH. The ultraviolet spectra were given for many of the compds. given above. The screening of these compds. against tumors in mice thus far has not revealed any significant antitumor agents in this series.